=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 17:05:26 ON 07 OCT 2000
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

FILE COVERS 1967 - 7 Oct 2000 VOL 133 ISS 16
FILE LAST UPDATED: 6 Oct 2000 (20001006/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

This file supports REGlstRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

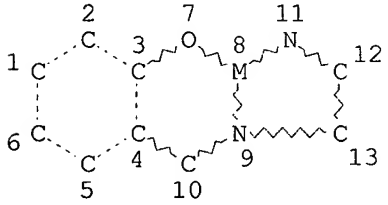
Now you can extend your author, patent assignee, patent information, and title searches back to 1907. The records from 1907-1966 now have this searchable data in CAOLD. You now have electronic access to all of CA: 1907 to 1966 in CAOLD and 1967 to the present in HCAPLUS on STN.

=>

=>

=> d stat que l25

L5 STR

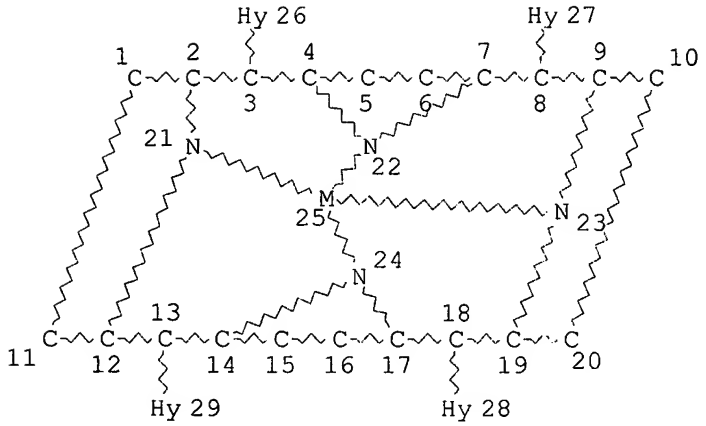


NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE
L7 18360 SEA FILE=REGISTRY SSS FUL L5
L12 STR

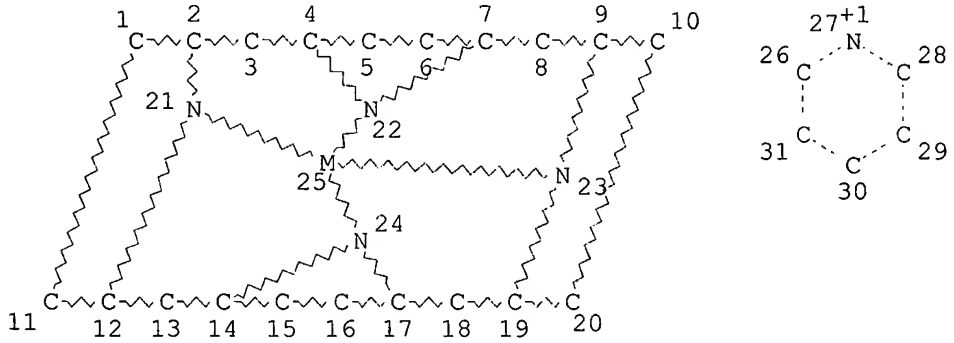
Checked JSL 9-25-2006

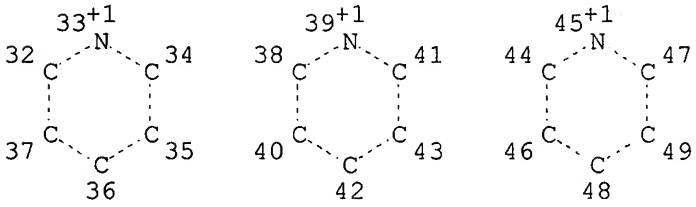


NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE
L14 STR





NODE ATTRIBUTES:
CHARGE IS E+1 AT 27
CHARGE IS E+1 AT 33
CHARGE IS E+1 AT 39
CHARGE IS E+1 AT 45
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 49

STEREO ATTRIBUTES: NONE
L17 988 SEA FILE=REGISTRY SSS FUL L12 AND L14
L23 5172 SEA FILE=HCAPLUS ABB=ON PLU=ON L7

```
L24         895 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L17
L25           4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L23 AND L24


=>

=>

=> d ibib abs hitrn l25 1-4


L25  ANSWER 1 OF 4  HCAPLUS  COPYRIGHT 2000 ACS
ACCESSION NUMBER:         1996:265572  HCAPLUS
DOCUMENT NUMBER:          124:310498
TITLE:                    Similarities and differences in the DNA
                          binding/cleaving specificities and mechanisms of
                          [SalenMn(III)]+ and [TMPPMn(III)]5+
AUTHOR(S):                Gravert, Dennis J.; Griffin, John H.
CORPORATE SOURCE:         Dep. Chem., Stanford Univ., Stanford, CA, 94305-5080,
                          USA
SOURCE:                   Bioorg. Med. Chem. Lett. (1996), 6(7), 889-92
                          CODEN: BMCLE8; ISSN: 0960-894X
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
AB   Affinity cleaving anal. reveals that [SalenMn(III)]+ (1) and
     [TMPPMn(III)]5 (2) exhibit nearly indistinguishable DNA double strand
     binding/cleaving specificities.  At nucleotide resoln., the complexes
     generate distinct patterns of cleavage within shared A:T rich target
     sequences.  DNA end product anal. indicates that 1 and 2 produce oxidative
     cleavage through both common and different mechanisms.
IT   47111-14-8 70649-54-6
     RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process);
     PROC (Process); USES (Uses)
        (similarities and differences in DNA binding/cleaving specificities and
        mechanisms of N,N'-ethylenebis(salicylideneaminato) manganese
        [SalenMn(III)]+ and meso-tetrakis(4-N-methylpyridiniumyl)porphyrinato
        manganese [TMPPMn(III)]5+)

L25  ANSWER 2 OF 4  HCAPLUS  COPYRIGHT 2000 ACS
ACCESSION NUMBER:         1996:110357  HCAPLUS
DOCUMENT NUMBER:          124:135707
TITLE:                    Pharmaceutical use of transition metal complexes as
                          peroxynitrite decomposition catalysts
INVENTOR(S):              Stern, Michael Keith; Salvemini, Daniela
PATENT ASSIGNEE(S):       Monsanto Co., USA
SOURCE:                   PCT Int. Appl., 68 pp.
                          CODEN: PIXXD2
DOCUMENT TYPE:            Patent
LANGUAGE:                 English
FAMILY ACC. NUM. COUNT:   1
PATENT INFORMATION:

     PATENT NO.        KIND  DATE          APPLICATION NO.  DATE
     ----------------  ----  --------      ---------------  --------
     WO 9531197         A1   19951123      WO 1995-US5886   19950509
         W:  AM, AU, BB, BG, BR, BY, CA, CN, CZ, EE, FI, GE, HU, IS, JP, KG,
             KR, KZ, LK, LR, LT, LV, MD, MG, MN, MX, NO, NZ, PL, RO, RU, SG,
             SI, SK, TJ, TM, TT, UA, US, UZ, VN
         RW: KE, MW, SD, SZ, UG, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT,
             LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE,
             SN, TD, TG
     CA 2189528         AA   19951123      CA 1995-2189528  19950509
     AU 9525120         A1   19951205      AU 1995-25120    19950509
     AU 709553          B2   19990902
     EP 758892          A1   19970226      EP 1995-919143   19950509
         R:  AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, NL, PT, SE
```

CN 1152871	A	19970625	CN 1995-194075	19950509
HU 76327	A2	19970828	HU 1996-3140	19950509
BR 9507643	A	19970923	BR 1995-7643	19950509
JP 10500671	T2	19980120	JP 1995-529755	19950509
NO 9604793	A	19970106	NO 1996-4793	19961112
FI 9604537	A	19970110	FI 1996-4537	19961112
PRIORITY APPLN. INFO.:			US 1994-242498	19940513
			WO 1995-US5886	19950509

OTHER SOURCE(S): MARPAT 124:135707

AB Diseases assocd. with the decompn. of peroxynitrite (formed in the body by interaction of metabolically produced NO with superoxide) are ameliorated by treatment with transition metal complexes (e.g. with porphyrins or macrocyclic N compds.) which accelerate decompn. of peroxynitrite, preferably to benign products. Diseases which may thus be treated include ischemic reperfusion, inflammation, sepsis, stroke, multiple sclerosis, parkinsonism, and side effects from cancer chemotherapy. The complexes prevent tissue damage from decompn. of peroxynitrite to toxic HO.bul. and NO2, and also protect superoxide dismutase from inactivation. Thus, intestinal vascular leakage in rats during endotoxin shock, measured as leakage of 125I-labeled serum albumin, was lessened by i.v. injection of acetato[5,10,15,20-tetrakis(N-methyl-4-pyridyl)porphinato]iron(III) tetratosylate (30 mg/kg) 3 h after lipopolysaccharide injection.

IT **62945-14-6P 173443-75-9P**

RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(pharmaceutical use of transition metal complexes as peroxynitrite decompn. catalysts)

L25 ANSWER 3 OF 4 HCAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER:	1995:308976 HCAPLUS
DOCUMENT NUMBER:	122:132480
TITLE:	Kinetic Control of Reactions of Electrogenerated Co(I) Macrocycles with Alkyl Bromides in a Bicontinuous Microemulsion
AUTHOR(S):	Zhou, De-ling; Gao, Jianxin; Rusling, James F.
CORPORATE SOURCE:	Department of Chemistry, University of Connecticut, Storrs, CT, 06269-3060, USA
SOURCE:	J. Am. Chem. Soc. (1995), 117(3), 1127-34 CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE:	Journal
LANGUAGE:	English

AB Bicontinuous microemulsions made from dodecane, water, and didodecyldimethylammonium bromide (DDAB) were investigated as media for the catalytic redn. of trans-1,2-dibromocyclohexane (DBCH) and for SN2 reactions of n-alkyl bromides with electrochem. generated Co(I) complexes. Macrocyclic complexes vitamin B12 (a cobalt corrin) and Co(salen) resided in the water phase, while the alkyl bromides resided in the oil phase of the microemulsion. Rates of these bimol. reactions were comparable in bicontinuous microemulsions to those in homogeneous solvents. Rates of DBCH redn. 40-fold larger in the bicontinuous fluid than that in a water-in-oil microemulsion may be caused by a larger interfacial area of the bicontinuous system. For a given alkyl halide, a linear relation between log k1 and E.degree.'Co(II)/Co(I) was found for both catalytic and SN2 reactions for rate consts. in DMF and the microemulsion. Thus, kinetic differences are controlled by activation free energies governed mainly by the formal potential of the Co(II)/Co(I) redox couple, rather than by distribution of reactants between phases. Formal potentials in the microemulsion depended on specific interactions, such as those of CoI(salen)- with cationic surfactant head groups or the influence of water phase pH on vitamin B12.

IT **79346-65-9**

RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process)

(kinetic control of SN2 reactions of electrogenerated Co(I) macrocycles with alkyl bromides in a bicontinuous microemulsion)

IT **14167-18-1**, Co(salen)
RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process); USES (Uses)
(kinetic control of reactions of electrogenerated Co(I) macrocycles with alkyl bromides in a bicontinuous microemulsion)

L25 ANSWER 4 OF 4 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1991:246585 HCAPLUS
DOCUMENT NUMBER: 114:246585
TITLE: Porphinatoiron-catalyzed oxygenation of styrene in aqueous solution
AUTHOR(S): Kano, Koji; Takagi, Hiroyuki; Takeuchi, Masayuki; Hashimoto, Shizunobu; Yoshida, Zenichi
CORPORATE SOURCE: Fac. Eng., Doshisha Univ., Kyoto, 602, Japan
SOURCE: Chem. Lett. (1991), (3), 519-22
CODEN: CMLTAG; ISSN: 0366-7022
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A quant. oxygenation of styrene to 1-phenylethanol is realized in a reaction catalyzed by an Fe complex of 5,10,15,20-tetrakis(1-methyl-4-pyridinio)porphine tetrachloride (FeTMPyP) in water contg. NaBH4. A plausible mechanism involving a styrene carbanion stabilized by Fe(III)TMPyP as an intermediate is presented.
IT **14167-18-1**
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for oxygenation of styrene)
IT **126425-09-0**
RL: CAT (Catalyst use); USES (Uses)
(catalysts, for oxygenation of styrene and related compds.)

=> select hit rn l25 1-4

E1 THROUGH E7 ASSIGNED

=>

=>

=> fil reg

FILE 'REGISTRY' ENTERED AT 17:06:39 ON 07 OCT 2000
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

STRUCTURE FILE UPDATES: 6 OCT 2000 HIGHEST RN 293726-17-7
DICTIONARY FILE UPDATES: 6 OCT 2000 HIGHEST RN 293726-17-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 11, 2000

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT for details.

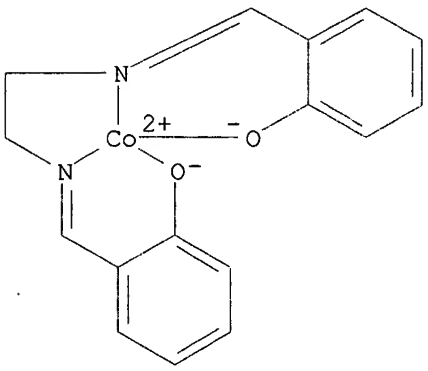
=>

=>

=> d his l26

(FILE 'HCAPLUS' ENTERED AT 17:05:26 ON 07 OCT 2000)
SELECT HIT RN L25 1-4

LC STN Files: BIOBUSINESS, BIOSIS, CA, CAOLD, CAPLUS, CASREACT, CHEMCATS, CHEMLIST, CSCHEM, GMELIN*, HSDB*, IFICDB, IFIPAT, IFIUDB, MEDLINE, MSDS-OHS, PIRA, RTECS*, TOXLINE, TOXLIT, USPATFULL
(*File contains numerically searchable property data)
Other Sources: EINECS**, NDSL**, TSCA**
(**Enter CHEMLIST File for up-to-date regulatory information)



548 REFERENCES IN FILE CA (1967 TO DATE)
29 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
549 REFERENCES IN FILE CAPLUS (1967 TO DATE)
12 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

REFERENCE 1: 133:208327

REFERENCE 2: 133:184636

REFERENCE 3: 133:136275

REFERENCE 4: 133:114133

REFERENCE 5: 133:114101

REFERENCE 6: 133:104592

REFERENCE 7: 133:89616

REFERENCE 8: 133:65202

REFERENCE 9: 133:22947

REFERENCE 10: 132:309344

=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 17:11:31 ON 07 OCT 2000
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2000 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications.

FILE COVERS 1967 - 7 Oct 2000 VOL 133 ISS 16
FILE LAST UPDATED: 6 Oct 2000 (20001006/ED)

This file contains CAS Registry Numbers for easy and accurate

substance identification.

This file supports REG1stRY for direct browsing and searching of all substance data from the REGISTRY file. Enter HELP FIRST for more information.

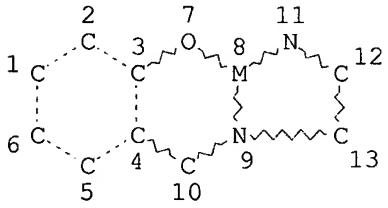
Now you can extend your author, patent assignee, patent information, and title searches back to 1907. The records from 1907-1966 now have this searchable data in CAOLD. You now have electronic access to all of CA: 1907 to 1966 in CAOLD and 1967 to the present in HCAPLUS on STN.

=>

=>

=> d stat que l32

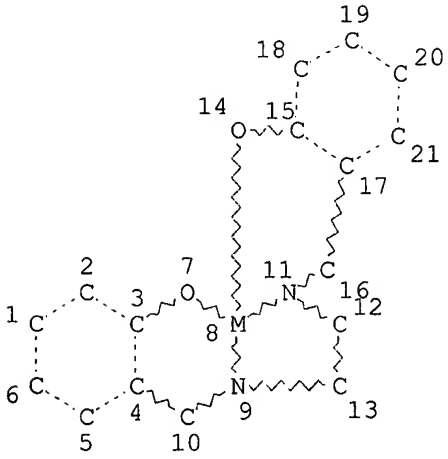
L5 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE
L7 18360 SEA FILE=REGISTRY SSS FUL L5
L8 STR

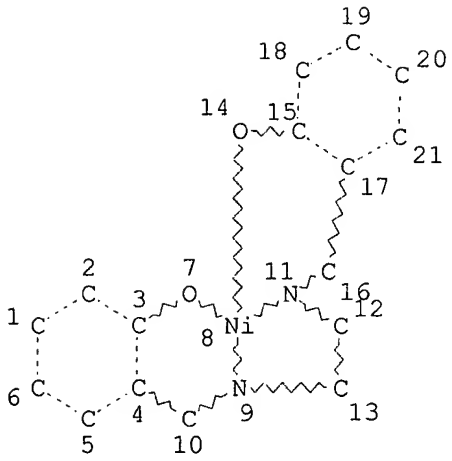


NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE
L9 5204 SEA FILE=REGISTRY SUB=L7 SSS FUL L8

L10 STR



NODE ATTRIBUTES:
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE

```
L11          484 SEA FILE=REGISTRY SUB=L9 SSS FUL L10
L20          418 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L11
L27            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  DNA/CN
L28              SEL  PLU=ON  L27 1- CHEM :        4 TERMS
L29       482681 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L28
L30       544802 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L29 OR DNA OR ?DEOXYRIBONU?
L31       528726 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L30 NOT (?DNASE? OR DNASE?)
L32            6 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20 AND L31
```

=>

=>

=> d ibib abs hitrn l32 1-6

L32 ANSWER 1 OF 6 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1999:757868 HCAPLUS
DOCUMENT NUMBER: 132:104228
TITLE: Nickel and Cobalt Reagents Promote Selective Oxidation of Z-**DNA**
AUTHOR(S): Tang, Ning; Muller, James G.; Burrows, Cynthia J.; Rokita, Steven E.
CORPORATE SOURCE: Department of Chemistry and Biochemistry, University of Maryland, College Park, MD, 20742, USA
SOURCE: Biochemistry (1999), 38(50), 16648-16654
CODEN: BICHAW; ISSN: 0006-2960
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The structural characteristics of Z-**DNA** were used to challenge the selectivity of guanine oxidn. promoted by nickel and cobalt reagents. Base pairing and stacking within all helical structures studied previously had hindered access to guanine and limited its reaction. However, the Z-helix uniquely retains high exposure of guanine N7. This exposure was sufficient to direct oxidn. specifically to a plasmid insert -(CG)13AATT(CG)13- that adopted a Z-conformation under native

supercoiling. An alternative insert -(CG)7- retained its B-conformation and demonstrated the expected lack of reactivity. For a nickel salen complex made from a particularly bulky ligand, preferential reaction shifted to the junctions within the Z-**DNA** insert as is common for large reagents. Inactivation of the nickel reagents by high-salt concns. prevented parallel investigations of Z-**DNA**, formed by oligonucleotides. However, the activity of Co2+ was minimally affected by salt and consequently confirmed the high reactivity of 5'-p(CG)4 in its Z-conformation. These reagents may now be applied to a broad array of targets, since their structural specificity remains predictable for both complex and helical assemblies of nucleic acids.

IT **152921-10-3**
RL: RCT (Reactant)
(nickel and cobalt reagents promote selective oxidn. of Z-**DNA**
)

REFERENCE COUNT: 64
REFERENCE(S):
(1) Abrescia, N; Nucleic Acids Res 1999, V27, P1593 HCAPLUS
(2) Burrows, C; Acc Chem Res 1994, V27, P295 HCAPLUS
(3) Burrows, C; Chem Rev 1998, V98, P1109 HCAPLUS
(4) Burrows, C; Metal Ions in Biological Systems 1996, P537 HCAPLUS
(5) Butcher, S; J Mol Biol 1994, V244, P52 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L32 ANSWER 2 OF 6 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1997:56325 HCAPLUS
DOCUMENT NUMBER: 126:168729
TITLE: Highly preferential cleavage of unpaired guanines in **DNA** by a functionalized salen-nickel complex
AUTHOR(S): Routier, Sylvain; Bernier, Jean-Luc; Catteau, Jean-Pierre; Gailly, Christian
CORPORATE SOURCE: Lab. Chimie Organique Physique, URA CNRS, Villeneuve, 59655, Fr.
SOURCE: Bioorg. Med. Chem. Lett. (1997), 7(1), 63-66
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In the presence of oxygen donor compds., a functionalized salen-nickel complex poorly cuts double-stranded **DNA** but induces strong cleavages at guanine residues in the single-stranded region of hairpin oligonucleotides.
IT **182931-32-4P**
RL: NUU (Nonbiological use, unclassified); SPN (Synthetic preparation); PREP (Preparation); USES (Uses)
(highly preferential cleavage of unpaired guanines in **DNA** by a functionalized salen-nickel complex)
IT **182931-29-9P**
RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation)
(highly preferential cleavage of unpaired guanines in **DNA** by a functionalized salen-nickel complex)

L32 ANSWER 3 OF 6 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1996:27196 HCAPLUS
DOCUMENT NUMBER: 124:169908
TITLE: Ambient oxygen activating water soluble cobalt-salen complex for **DNA** cleavage
AUTHOR(S): Bhattacharya, Santanu; Mandal, Subhrangsu S.
CORPORATE SOURCE: Department Organic Chemistry, Indian Institute Science, Bangalore, 560012, India
SOURCE: J. Chem. Soc., Chem. Commun. (1995), (24), 2489-90
CODEN: JCCCAT; ISSN: 0022-4936
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A new water-sol. CoII-salen complex cleaves **DNA** spontaneously

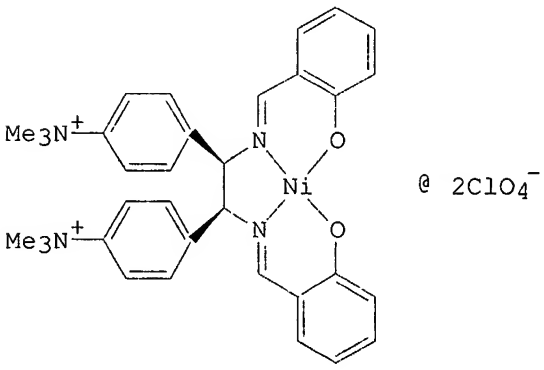
under ambient aerobic conditions; the cleavage is further enhanced by inclusion of 2 mmol/dm3 dithiothreitol in the reaction buffer.

IT **173482-00-3**
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(**DNA** cleavage by ambient oxygen-activating water-sol. cobalt-salen complex)

L32 ANSWER 4 OF 6 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1995:250101 HCAPLUS
DOCUMENT NUMBER: 122:48840
TITLE: **DNA** modification promoted by water-soluble nickel(II) salen complexes: a switch to **DNA** alkylation
AUTHOR(S): Muller, James G.; Paikoff, Sari J.; Rokita, Steven E.; Burrows, Cynthia J.
CORPORATE SOURCE: Dep. Chem., State Univ. New York, Stony Brook, Stony Brook, NY, USA
SOURCE: J. Inorg. Biochem. (1994), 54(3), 199-206
CODEN: JIBIDJ; ISSN: 0162-0134
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Reaction of a 17-base hairpin-forming oligonucleotide with [N,N'-bis(salicylaldehyde)-meso-1,2-bis(4-trimethylaminophenyl)ethylenediimino]nickel(II) perchlorate and KHSO5 produced two types of high mol. wt. products, an alk.-labile species and a nonalkaline-labile species, which co-migrated on gel electrophoresis. Upon treatment with piperidine, the base-labile deriv. led to strand scission products only at accessible guanine residues that were not part of a Watson-Crick duplex. The formation of higher mol. wt. species is proposed to occur via a highly reactive ligand-centered radical acting as a **DNA** alkylating agent.

IT **152921-09-0**
RL: ADV (Adverse effect, including toxicity); BPR (Biological process); BIOL (Biological study); PROC (Process)
(nickel(II) complexes synthesis and **DNA** modification)

L32 ANSWER 5 OF 6 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1994:128946 HCAPLUS
DOCUMENT NUMBER: 120:128946
TITLE: A primer extension assay for modification of guanine by nickel(II) complexes
AUTHOR(S): Woodson, Sarah A.; Muller, James G.; Burrows, Cynthia J.; Rokita, Steven E.
CORPORATE SOURCE: Dep. Chem. Biochem., Univ. Maryland, College Park, MD, 20742-2021, USA
SOURCE: Nucleic Acids Res. (1993), 21(23), 5524-5
CODEN: NARHAD; ISSN: 0305-1048
DOCUMENT TYPE: Journal
LANGUAGE: English
GI



I

AB To generate reliable structural information, it is advantageous to use a variety of reagents with differing specificities. To this end the authors have developed a new inorg. probe for nucleic acid structure. In particular, guanine is selectively oxidized by a planar Ni complex (I) in the presence of KHSO5. The extent to which guanines in oligodeoxynucleotides and yeast tRNAPhe are modified by I correlates well with the solvent accessibility of guanine N7. The utility of this reagent for RNA structure has been further demonstrated by its application to the Tetrahymena intron.

IT **152921-10-3**
RL: RCT (Reactant)
(guanine oxidn. by, in RNA and **DNA** structure anal.)

L32 ANSWER 6 OF 6 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1992:648070 HCAPLUS
DOCUMENT NUMBER: 117:248070
TITLE: Cleavage of **DNA** by nickel complexes
AUTHOR(S): Morrow, Janet R.; Kolasa, Kimberly A.
CORPORATE SOURCE: Dep. Chem., State Univ. New York, Buffalo, NY, 14214, USA
SOURCE: Inorg. Chim. Acta (1992), 195(2), 245-8
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The cleavage of plasmid **DNA** (pUB110) by several square planar nickel(II) complexes in the presence of either magnesium monoperoxyphthalic acid (MPPA) or iodosylbenzene was investigated. At 25.degree. and near neutral pH, Ni(salen) (100 .mu.M) or Ni(CR)2+ (100 .mu.M) promoted complete conversion of supercoiled plasmid to the nicked circular form in 5 min with iodosylbenzene (0.1 g/mL) as oxidant or in 2.5 h with MPPA (1 mM) as oxidant (salen = bis(salicylaldehyde)ethylenediimine, CR = 2,12-dimethyl-2,3,11,17-tetraazabicyclo[11.3.1]heptadeca-1(17),2,11,13,15-pentaene). No cleavage was obsd. under similar conditions with Ni(cyclam)2+, Ni(dioxocyclam), Ni(TPP) or Ni(NO3)2 (cyclam = 1,4,8,11-tetraazacyclotetradecane, dioxocyclam = 1,4,8,11-tetraazacyclotetradecane-5,7-dione, TPP = 5,10,15,20-tetraphenyl-21H,23H-porphine). Possible roles for the nickel complexes in promoting **DNA** cleavage are discussed.

IT **14167-20-5**
RL: ANST (Analytical study)
(**DNA** cleavage promoted by, in presence of oxidizing agents, nickel complex role in)

=> d stat que l37 nos

L5		STR
L7	18360	SEA FILE=REGISTRY SSS FUL L5
L8		STR
L9	5204	SEA FILE=REGISTRY SUB=L7 SSS FUL L8
L10		STR
L11	484	SEA FILE=REGISTRY SUB=L9 SSS FUL L10
L12		STR
L14		STR
L17	988	SEA FILE=REGISTRY SSS FUL L12 AND L14
L20	418	SEA FILE=HCAPLUS ABB=ON PLU=ON L11
L23	5172	SEA FILE=HCAPLUS ABB=ON PLU=ON L7
L24	895	SEA FILE=HCAPLUS ABB=ON PLU=ON L17
L25	4	SEA FILE=HCAPLUS ABB=ON PLU=ON L23 AND L24
L33	8	SEA FILE=HCAPLUS ABB=ON PLU=ON L20 AND ?NUCLEIC?(5A)ACID
L36	14	SEA FILE=HCAPLUS ABB=ON PLU=ON L20 AND (?PROTEIN? OR AMINO(W)ACID OR AA OR ?PEPTID?)
L37	14	SEA FILE=HCAPLUS ABB=ON PLU=ON L36 NOT (L25 OR L33)

=>

=>

=> d ibib abs hitrn l37 1-14

L37 ANSWER 1 OF 14 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 2000:206635 HCAPLUS
DOCUMENT NUMBER: 132:231088
TITLE: Procedure for the preparation of transition metal complexes with bis(salicylidene)ethylenediamine or -o-phenylenediamine derivatives.
INVENTOR(S): Jaedicke, Hagen; Klatt, Martin Jochen; Ruff, Detlef
PATENT ASSIGNEE(S): BASF A.-G., Germany
SOURCE: Ger. Offen., 6 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 19843875	A1	20000330	DE 1998-19843875	19980925

OTHER SOURCE(S): MARPAT 132:231088
AB Procedures for the prepn. of transition metal complexes with bis(salicylidene)ethylenediamine or -o-phenylenediamine by the reaction of an unsubstituted or substituted (non)optically active salicylaldehyde with a (non)optically active diamine or amine at increased temp. in a suitable solvent, followed by reaction with a divalent transition metal oxide.
IT **14167-20-5P**, [Bis(salicylidene)ethylenediaminato]nickel
261623-86-3P
RL: IMF (Industrial manufacture); PREP (Preparation)
(prepn. from transition metal oxide and salicylaldehyde and diamine in suitable solvent)

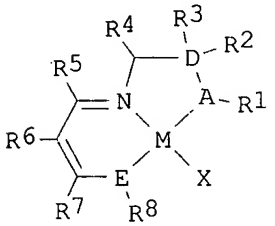
L37 ANSWER 2 OF 14 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1999:524514 HCAPLUS
DOCUMENT NUMBER: 131:286787
TITLE: Chiral salen-metal complexes as novel catalysts for asymmetric phase transfer alkylations
AUTHOR(S): Belokon, Yuri N.; North, Michael; Kublitski, Vadim S.; Ikonnikov, Nikolai S.; Krasik, Pavel E.; Maleev, Viktor I.
CORPORATE SOURCE: A.N.Nesmeyanov.Institute of Organo-Element Compounds, Russian Academy of Sciences, Moscow, 117813, Russia
SOURCE: Tetrahedron Lett. (1999), 40(33), 6105-6108
CODEN: TELEAY; ISSN: 0040-4039
PUBLISHER: Elsevier Science Ltd.
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 131:286787
AB Chiral, salen-metal complexes have been tested as catalysts for the C-alkylation of aldimine Schiff's bases of alanine esters with alkyl bromides under phase-transfer conditions (solid sodium hydroxide, toluene, ambient temp., 1-10% of the catalyst). The best catalyst, which was derived from a Cu(II) complex of (1R,2R or 1S,2S)-[N,N'-bis(2'-hydroxy-benzylidene)]-1,2-diamino-cyclohexane, gave .alpha.-methyl-.alpha.-**amino acids** with enantiomeric excesses of 70-96%.
IT **246047-02-9**
RL: CAT (Catalyst use); USES (Uses)
(use of as catalysts for asym. phase transfer alkylations in the prepn. of **amino acids**)
REFERENCE COUNT: 29

REFERENCE(S): (1) Amundsen, A; Inorg Chem 1979, V18, P206 HCAPLUS
(4) Belokon', Y; Izv Akad Nauk Ser Khim SSSR 1991, P126 HCAPLUS
(6) Belokon', Y; Tetrahedron: Asymmetry 1996, V7, P851 HCAPLUS
(7) Belokon', Y; Tetrahedron: Asymmetry 1998, V9, P851 HCAPLUS
(8) Chinchilla, R; Angew Chem Int Ed 1997, V36, P995 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

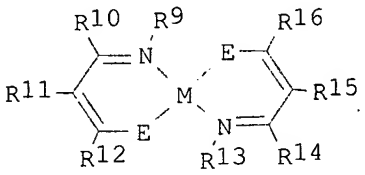
L37 ANSWER 3 OF 14 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1999:175688 HCAPLUS
DOCUMENT NUMBER: 130:191009
TITLE: Group 10 and 11 transition-metal Schiff-base complexes as cysteine protease inhibitors
INVENTOR(S): Grinstaff, Mark W.; Gray, Harry B.; Meade, Thomas J.
PATENT ASSIGNEE(S): California Institute of Technology, USA
SOURCE: U.S., 18 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 5880149	A	19990309	US 1996-721872	19960927

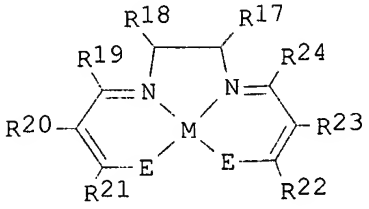
OTHER SOURCE(S): MARPAT 130:191009
GI



I



II



III

AB The invention relates to a variety of Group 10 and 11 transition-metal Schiff-base complexes used to bind **proteins** and enzymes. Claims and examples include complexes I [M = Cu, Ag, Au, Ni, Pd, Pt; A = N or O; E = O, N, S, or Se; D = C, B, or P; R1-R8 = a variety of groups, e.g., H, halo, alkyl, alc., amine, etc.; X = counterion or neutral coordinating ligand]. Further provided in the summary with examples are complexes II [same M as above; E = O, S, Se; R9-R16 = a variety of groups, e.g., H, halo, alkyl, alc., amine, etc.] and complexes III [same M as above,; E = O, S, Se; R17-R24 = a variety of groups, e.g., H, halo, alkyl, alc., amine, etc.]. Pharmaceutical compns. comprising I in an admixt. with a

pharmaceutically acceptable carrier are claimed (no examples). Complexes I are cysteine protease inhibitors, and as such may be used in the treatment of disorders assocd. with cysteine protease.

IT **14167-20-5P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(prepn. as cysteine protease inhibitor and for treatment of disorders assocd. with cysteine protease)

REFERENCE COUNT: 18
REFERENCE(S):
(1) Becker, M; Kinetics of Ligand Substitution in Platinum(II) Complexes:A Study on the Concept of Nucleophillic Discrimination 1966, 22, P750 HCAPLUS
(2) Chakraborty, H; Catalytic Activities of Schiff Base Aquocomplexes of Copper(ii) in the Hydrolysis of Amino Esters 1995, 7, P1154 HCAPLUS
(3) Costes; Inorganica Chimica Acta 1995, V237(1-2), P57 HCAPLUS
(4) Defilippo, D; Silver and Gold(I) Complexes with Thiomorpholin-3-One Kinetics of Reduction of Gold(III) 1971, 6, P315 HCAPLUS
(6) Elo, H; Corelation Between Reactivity and Biological Activity" 1987, 18, P918 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 4 OF 14 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1999:114715 HCAPLUS
DOCUMENT NUMBER: 130:245617
TITLE: **Protein** Engineering: Design of Single-Residue-Anchored Metal-Uptake Systems
AUTHOR(S): Ranganathan, Subramania; Tamilarasu, Natarajan
CORPORATE SOURCE: Biomolecular Research Unit, Regional Research Laboratory, Trivandrum, 695 019, India
SOURCE: Inorg. Chem. (1999), 38(5), 1019-1023
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
GI

* STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

AB Ethylenediamine-acetylacetone mono-Schiff base (AEH), hydroxylamine hydrochloride and ethylenediamine readily condense with **peptides** having 3-acetyltyrosine side chains to templates having two types of structural profile with AEH, hydroxylamine hydrochloride and ethylenediamine requiring two **peptide** units. Oximes I (R = Bz, R1 = OMe; R = Boc-Ala, R1 = OMe, Ser-OMe) were prepd. by the oximation of the corresponding 3-acetyltyrose derivs. with hydroxylamine hydrochloride, whereas Schiff bases II and III (R, R1 = same) were prepd. by treating the corresponding 3-acetyltyrose derivs. with ethylenediamine-acetylacetone mono-Schiff base and ethylenediamine, resp. I, II and III were complexed with transition metals to give the corresponding complexes.

IT **221236-53-9P 221236-70-0P 221236-90-4P**
221237-04-3P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of)

REFERENCE COUNT: 35
REFERENCE(S):
(1) Boger, D; J Org Chem 1987, V52, P5283 HCAPLUS
(4) Costes, J; Inorg Chim Acta 1982, V60, P111 HCAPLUS
(5) de Tar, D; J Am Chem Soc 1967, V89, P3039 HCAPLUS
(12) Ito, N; Nature 1991, V350, P87 HCAPLUS

(16) Pettit, G; J Chem Soc, Perkin Trans 1 1973, P950
HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L37 ANSWER 5 OF 14 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1998:382298 HCAPLUS
DOCUMENT NUMBER: 129:130869
TITLE: Inhibition of human cytomegalovirus **proteinase** by salcomine derivatives
AUTHOR(S): Watanabe, S.; Konno, K.; Shigeta, S.; Yokota, T.
CORPORATE SOURCE: Rational Drug Design Laboratories, Fukushima, 960-12, Japan
SOURCE: Antiviral Chem. Chemother. (1998), 9(3), 269-274
CODEN: ACCHEH; ISSN: 0956-3202
PUBLISHER: International Medical Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Salcomine, N,N'-bis(salicylidene)ethylene diaminocobalt (II), and its derivs. were evaluated for their ability to inhibit selectively human cytomegalovirus (HCMV) **proteinase** activity. The 50% inhibitory concn. (IC50) of salcomine was 1.4 .mu.M for HCMV **proteinase**, but >200 .mu.M for three other serine **proteinases** (trypsin, >250 .mu.M; chymotrypsin, 206 .mu.M; and elastase, >250 .mu.M). Two salcomine derivs. also inhibited HCMV **proteinase** with IC50 values under 2 .mu.M. Studies of the structure-activity relationship of salcomine-related compds. showed that the Ph moiety and the spacer moiety (distance between the two amines) were instrumental in the inhibition of HCMV **proteinase**. Moreover, salcomine inhibited the growth of lab. strain AD169 and three clin. isolates at a 50% effective concn. (EC50) range of 1.92-2.89 .mu.M. These results show that salcomine derivs. are potent and selective inhibitors of HCMV **proteinase** and HCMV replication in cell culture. Salcomine derivs. appear to be worth pursuing as candidate drugs for the chemotherapy of HCMV infection.
IT **14167-20-5**
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(salcomine derivs. structure-related inhibition of human cytomegalovirus **proteinase**)

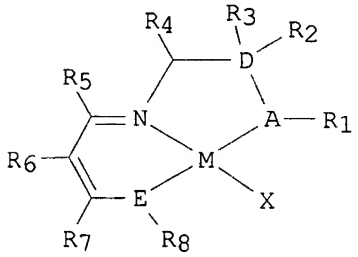
L37 ANSWER 6 OF 14 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1997:651396 HCAPLUS
DOCUMENT NUMBER: 127:287194
TITLE: Application of microwave heating techniques for the solid state reactions of coordination compounds. (I). Synthesis of Co(II), Ni(II) and Cu(II) complexes by solid state reactions under microwave
AUTHOR(S): Jia, Dian-Zeng; Yang, Li-Xin; Xia, Xi; Xin, Xin-Quan
CORPORATE SOURCE: Dep. Chem., Xinjiang Univ., Urumqi, 830046, Peop. Rep. China
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (1997), 18(9), 1432-1435
CODEN: KTHPDM; ISSN: 0251-0790
PUBLISHER: Gaodeng Jiaoyu Chubanshe
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB Solid-state reactions of the transition metal acetates Co(OAc)2.cntdot.4H2O, Ni(OAc)2.cntdot.4H2O, and Cu(OAc)2.cntdot.H2O with org. compds. such as **amino acids** (glycine and DL-alanine), Schiff bases [N,N'-di(salicylidene)ethylenediamine (H2SB1) and N,N'-di(salicylidene)-o-phenylenediamine (H2SB2)], .beta.-diketone [keto and enol forms of 1-phenyl-3-methyl-4-benzoyl-5-pyrazolone (HPMBP)], and 8-hydroxyquinoline (Hoxine) were studied in the microwave oven. The coordination compds. can be synthesized by solid state reactions up to 50 times faster in a microwave oven than by conventional techniques. The results suggest a significant potential value of microwave heating in solid state coordination chem.
IT **14167-20-5P**, [Bis(salicylidene)ethylenediaminato]nickel

RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. by solid-state reaction under microwave heating)

L37 ANSWER 7 OF 14 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1997:308082 HCAPLUS
DOCUMENT NUMBER: 126:287179
TITLE: Metal complexes as cysteine protease inhibitors
INVENTOR(S): Grinstaff, Mark W.; Gray, Henry B.; Meade, Thomas J.
PATENT ASSIGNEE(S): California Institute of Technology, USA
SOURCE: PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9711950	A1	19970403	WO 1996-US15527	19960927
W: AU, CA, IL, JP				
RW: AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE				
CA 2232821	AA	19970403	CA 1996-2232821	19960927
AU 9673767	A1	19970417	AU 1996-73767	19960927
EP 862574	A1	19980909	EP 1996-936017	19960927
R: AT, BE, CH, DE, DK, FR, GB, IT, LI, NL, SE				
JP 11513381	T2	19991116	JP 1996-513680	19960927
PRIORITY APPLN. INFO.:			US 1995-4451	19950928
			WO 1996-US15527	19960927

OTHER SOURCE(S): MARPAT 126:287179
GI



I

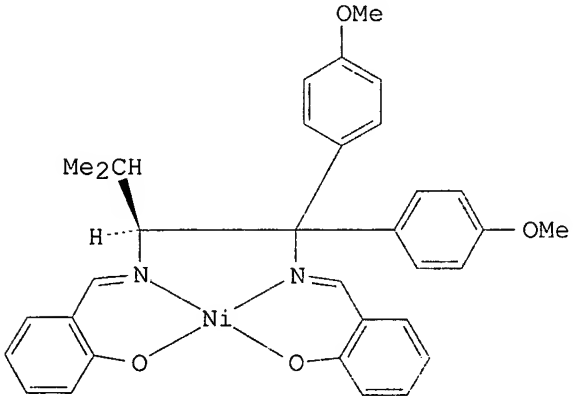
AB The invention relates to the prepn. of metal complexes (I) and related imine complexes used to bind **proteins** and enzymes, where M = Cu, Ag, Au, Ni, Pd or Pt; A = N or O; E = O, S, N or Se; D = C, B, P; X = a counterion or a neutral coordinating ligand; R1, R2, R3, R4, R5, R6, R7, R8 = H, halogen, alkyl, alkyl alc., alc., alkyl thiol, alkyl acid, alkyl amine, amine, aryl, a targeting moiety; R1 may also be absent when A is oxygen, S, or Se; R2 may also be carbonyl oxygen, phosphonyl oxygen, or -OR5 when A is boron; R3 can also be -OR5 when A is boron or phosphorus, or absent when R2 is carbonyl oxygen; R6R7 = cycloalkyl, aryl; R8 may also be absent when E is oxygen, sulfur or selenium. Addnl., MLX (M = Cu, Ag, Au; L = hydrotris(pyrazolyl)borate deriv.), M(RR'CHSR'')X (M = Cu, Ag, Au, Ni, Pd, Pt), MLX2 (M = Cu, Ni, Pd, Pt; L = ethylenediamine deriv. or malonic acid deriv.). Thus, [CuLCl] was prepd. from salicylaldehyde, N-ethylethylenediamine and CuCl2 and was shown to nearly completely inhibit papain enzyme after 1 h (10 .mu.M enzyme, 25 .mu.M metal inhibitor).

IT **14167-20-5P**
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(prepn. of metal complexes as cysteine protease inhibitors)

L37 ANSWER 8 OF 14 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1996:316370 HCAPLUS
DOCUMENT NUMBER: 125:51912
TITLE: Antioxidative activity of biologically active compounds: Measurement by Cypridina chemiluminescence method
AUTHOR(S): Suzuki, N.; Mashiko, S.; Hamada, M.; Nomoto, T.; Hasegaga, M.; Yoda, B.
CORPORATE SOURCE: National University Fisheries, Shimonoseki, 759-65, Japan
SOURCE: Biolumin. Chemilumin., Proc. Int. Symp., 8th (1994), 219-222. Editor(s): Campbell, Andrew Keith; Kricka, Larry J.; Stanley, Philip E. Wiley: Chichester, UK. CODEN: 62UZAR
DOCUMENT TYPE: Conference
LANGUAGE: English
AB The highly sensitive Cypridina chemiluminescence method previously developed by the authors was used to det. the antioxidative activity of various **peptides** and salcomine derivs. **Proteins** from marine life showed 1-2 orders larger reaction rate consts. than did those from land animals and plants. Hydrolyzates of the **proteins** from land animals showed larger consts. than did the unhydrolyzed **proteins**. The salcomine derivs. were also strong antioxidants.
IT **14167-20-5**
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(antioxidative activity of biol. active compds.)

L37 ANSWER 9 OF 14 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1993:449862 HCAPLUS
DOCUMENT NUMBER: 119:49862
TITLE: Preparation of primary vicinal diamines from **amino acid** esters and crystal structure of a chiral nickel salen complex
AUTHOR(S): Wey, Shiow Jyi; O'Connor, Kenneth J.; Burrows, Cynthia J.
CORPORATE SOURCE: Dep. Chem., State Univ. New York, Stony Brook, NY, 11794-3400, USA
SOURCE: Tetrahedron Lett. (1993), 34(12), 1905-8
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 119:49862
GI



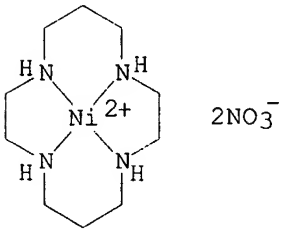
II

AB Highly pure chiral diamines (S)-H2NCHRC(C6H4OMe-4)2NH2 (I; R = CHMe2, Me)

were prepd. from H-L-Val-OMe.HCl and H-L-Ala-OEt.HCl in 4 steps. The x-ray crystal structure of the Ni(II) complex II derived from the bis-salicylaldehyde imine of I (R = CHMe2) reveals an interesting conformation around the metal center.

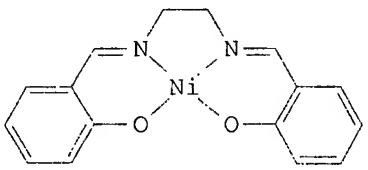
IT **148607-26-5P 148607-27-6P**
RL: PRP (Properties); SPN (Synthetic preparation); PREP (Preparation)
(prepn. and crystal structure of)

L37 ANSWER 10 OF 14 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1991:448614 HCAPLUS
DOCUMENT NUMBER: 115:48614
TITLE: Catalytic reactions of macrocyclic nickel(II) complexes
AUTHOR(S): Burrows, Cynthia J.
CORPORATE SOURCE: Dep. Chem., State Univ. New York, Stony Brook, NY, 11794-3400, USA
SOURCE: Inclusion Phenom. Mol. Recognit., [Proc. Int. Symp.], 5th (1990), Meeting Date 1988, 199-207. Editor(s): Atwood, Jerry L. Plenum: New York, N. Y.
CODEN: 57DUAJ
DOCUMENT TYPE: Conference
LANGUAGE: English
GI

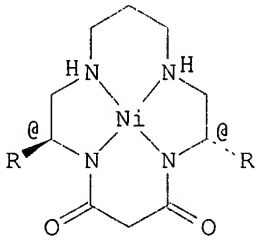


$2NO_3^-$

I



II



III

AB Symposium proceedings. Certain square planar Ni(II) complexes are active as catalysts for hydrocarbon oxidn. reactions including alkene epoxidn., oxidative C:C bond cleavage and hydroxylation. The reactions are highly dependent upon the structure of the ligand encapsulating Ni(II) and upon the terminal oxidant. Mechanistic studies of oxidns. using nickel-cyclam (I) and iodosylbenzene provide interesting comparisons with cytochrome P450 model catalysts. Higher turnover rates are obsd. with nickel-salen (II) as catalyst through the use of hypochlorite under phase transfer conditions. A third series of catalysts is based upon dioxocyclam complexes of Ni(II) (III) which are derived from **amino acids**. These complexes are effective with OCl- but not with PhIO.

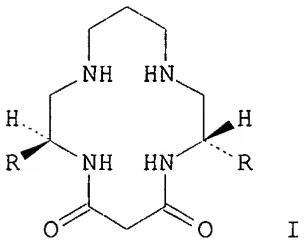
IT **14167-20-5**
RL: CAT (Catalyst use); USES (Uses)
(catalysts, contg. sodium hypochlorite, for epoxidn. of alkenes)

L37 ANSWER 11 OF 14 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1991:247798 HCAPLUS
DOCUMENT NUMBER: 114:247798

TITLE: Preparation of polyazamacrocycles and their metal complexes as phase-transfer epoxidation catalysts
INVENTOR(S): Burrows, Cynthia; Yoon, Heungsik; Wagler, Thomas R.
PATENT ASSIGNEE(S): State University of New York, Research Foundation, USA
SOURCE: U.S., 13 pp. Cont.-in-part of U.S. Ser. No. 261,032, abandoned.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4987227	A	19910122	US 1990-484102	19900223
US 5126464	A	19920630	US 1990-605249	19901029
US 5428180	A	19950627	US 1993-165063	19931210
PRIORITY APPLN. INFO.:			US 1988-261032	19881021
			US 1990-484102	19900223
			US 1990-605249	19901029
			US 1992-862728	19920403

OTHER SOURCE(S): CASREACT 114:247798; MARPAT 114:247798
GI



I

AB Azacrown compds. were prepd. by cyclocondensation of **amino acid** derivs. with diamines and diesters. Thus, macrocycles I (R = CH2Ph, CH2CHMe2, CHMe2) were prepd. by condensation of phenylalanine, leucine, and valine with 1,3-propanediamine followed by hydride redn. and cyclocondensation with di-Me malonate. Nickel complexes of I (R = CH2Ph, CH2CHMe2, CHMe2, H) were investigated as phase-transfer catalysts for the epoxidn. of (E)-PhCH:CHMe, norbornene, and cyclohexene.
IT **14167-20-5**
RL: CAT (Catalyst use); USES (Uses)
(catalyst, for epoxidn. of norbornene with hypochlorite)

L37 ANSWER 12 OF 14 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1991:7257 HCAPLUS
DOCUMENT NUMBER: 114:7257
TITLE: Preparation of cytotoxic LHRH analogs
INVENTOR(S): Schally, Andrew V.; Bajuz, Sandor; Janaky, Tamas
PATENT ASSIGNEE(S): Tulane Educational Fund, Inc., USA
SOURCE: Eur. Pat. Appl., 30 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 364819	A2	19900425	EP 1989-118460	19891005

EP 364819 A3 19910306
R: AT, BE, CH, DE, ES, FR, GB, GR, IT, LI, LU, NL, SE
JP 02157293 A2 19900618 JP 1989-273650 19891020
US 5258492 A 19931102 US 1991-710515 19910603
PRIORITY APPLN. INFO.: US 1988-260994 19881021
US 1989-404667 19890907
OTHER SOURCE(S): MARPAT 114:7257

AB R-X1-X2-X3-Ser-X5-X6-Q-Leu-Arg-Pro-X10-NH2 [I; R = H, alkanoyl, carbamyl; X1 = pyroglutamyl, Pro, D-3-(2-naphthyl)alanyl, D-4-chlorophenylalanyl; X2 = His, D-4-chlorophenylalanyl; X3 = Trp, D-Trp, D-3-(3-pyridyl)alanyl; X5 = Tyr, Arg; X6 = D-Phe, D-Lys, D-Orn, D-Phe(NH2); X10 = Gly, D-Ala; Q = bis-(2-chloroethyl)amino when X6 = D-Phe, or complexed metal contg. acyl, e.g., CH2(NH2)(CH2)m CH(NH2)(CH2)nCO[NH(CH2)oCO]p; m = 0, 1; n, p = 0-10; o = 1-10; metal = Pt, Ga, Ge, Sr, Ti, Va, Fe, Cu, Co, Au, Ni, Cd, Zn], were prepd. Thus, pGlu-His-Trp-Ser-Tyr-OH (pGlu = pyroglutamyl) and H-D-Mel-Leu-Arg-Pro-Gly-NH2.HCl [Mel = 4-[bis(2-chloroethyl)amino]-D-phenylalanyl] were coupled in DMF using (Me2CH)2NEt, DCC, and hydroxybenzotriazole at 0.degree. for 24 h to give [D-Mel6]LHRH. I at 1.5-10 .mu.g/rat showed 20-100% inhibition of ovulation.

IT **124010-85-1P 130585-14-7P 130694-92-7P**
130695-18-0P 130695-19-1P 130697-98-2P
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as cytotoxic LHRH analog)

L37 ANSWER 13 OF 14 HCAPLUS COPYRIGHT 2000 ACS

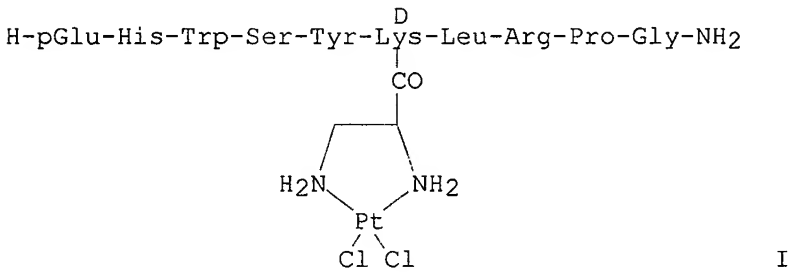
ACCESSION NUMBER: 1990:30731 HCAPLUS
DOCUMENT NUMBER: 112:30731

TITLE: Highly potent **metallopeptide** analogs of luteinizing hormone-releasing hormone

AUTHOR(S): Bajusz, S.; Janaky, T.; Csernus, V. J.; Bokser, L.; Fekete, M.; Srkalovic, G.; Redding, T. W.; Schally, A. V.
CORPORATE SOURCE: Sch. Med., Tulane Univ., New Orleans, LA, 70146, USA

SOURCE: Proc. Natl. Acad. Sci. U. S. A. (1989), 86(16), 6313-17
CODEN: PNASA6; ISSN: 0027-8424
DOCUMENT TYPE: Journal
LANGUAGE: English

GI



I

AB Metal complexes related to the cytotoxic complexes cisplatin and trans-bis(salicylaldoximato)copper(II) were incorporated into suitably modified LH-RH analogs contg. D-lysine at position 6. Some of the **metallopeptides** thus obtained proved to be highly active LH-RH agonists or antagonists. For instance, SB-40 (I) showed 50-fold higher LH-releasing potency than the native hormone. SB-95, [Ac-D-Nal(2)1,D-Phe(pCl)2,D-Pal(3)2,Arg5,D-Lys{DL-A2pr(Sal2Cu)}6,D-Ala10]LH-RH, where Nal(2) is 3-(2-naphthyl)alanine, Pal(3) is 3-(3-pyridyl)alanine, and Cu(II) is coordinated to the salicylideneimino moieties resulting from condensation of salicylaldehyde with D-Lys(DL-A2pr)6, caused 100% inhibition of ovulation at 3 .mu.g in rats. Most **metallopeptide** analogs of LH-RH showed high affinities for the membrane receptors of rat

pituitary and human breast cancer cells. Some of these **metallopeptides** had cytotoxic activity against human breast cancer and prostate cancer cell lines in vitro. Such cytostatic **metallopeptides** could be envisioned as targeted chemotherapeutic agents in cancers that contain receptors for LH-RH-like **peptides**
.

IT **123913-54-2P**, SB 106 **124010-85-1P**, SB 94
124086-37-9P, SB 101
RL: BAC (Biological activity or effector, except adverse); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn. and biol. activity of, structure in relation to)

L37 ANSWER 14 OF 14 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1981:582415 HCAPLUS
DOCUMENT NUMBER: 95:182415
TITLE: Transition metal complexes as catalysts in biochemical systems. Interaction with electron transfer processes
AUTHOR(S): Vol'pin, M. E.; Novodarova, G. N.; Kolosova, E. M.; Guzhova, N. V.; Kononenko, A. A.; Leikin, Yu. N.
CORPORATE SOURCE: Inst. Organoelem. Compounds, Moscow, 117334, USSR
SOURCE: Inorg. Chim. Acta (1981), 50(1), 21-31
CODEN: ICHAA3; ISSN: 0020-1693
DOCUMENT TYPE: Journal
LANGUAGE: English
AB It has been suggested that synthetic metal complexes can be used as catalysts for the regulation of certain processes in living cells. The complexes investigated were selected on the basis of their catalytic activity in model chem. reactions, such as autoxidn. of NADH, coenzyme Q4H2, and cytochrome c. Cobalt(II) complexes with 1,2,3,7,8,12,13,17,18,19-decamethyloctadehydrocorrin, N,N'-bis-(salicylidenyl)ethylenediamine, o-phenanthroline and other chelates proved to be active catalysts. The possibility of creating catalytic processes competing with the enzymic ones was tested exptl. by examples of this complex interaction with the mitochondrial respiratory chain and with the photosynthetic electron transfer system of purple bacteria. It was shown that some of the above-mentioned chem. catalysts of respiratory chain component autoxidn. could be integrated in electron transport at the subcellular level and could carry out catalytic electron transfer from coenzyme Q to O2 in mitochondria. Such a process competed with the enzymic one and was comparable with it in rate. Cobalt(II) tris-o-phenanthroline perchlorate interacted with the photosynthetic electron transfer system of purple bacteria, stimulating membrane energization in chromatophores.
IT **14167-20-5**
RL: BIOL (Biological study)
(NADH autoxidn. response to)

=> select hit rn l33 1-8;select hit rn l37 1-14

E1 THROUGH E10 ASSIGNED

E11 THROUGH E27 ASSIGNED

=> fil reg

FILE 'REGISTRY' ENTERED AT 17:18:27 ON 07 OCT 2000
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2000 American Chemical Society (ACS)

STRUCTURE FILE UPDATES: 6 OCT 2000 HIGHEST RN 293726-17-7
DICTIONARY FILE UPDATES: 6 OCT 2000 HIGHEST RN 293726-17-7

TSCA INFORMATION NOW CURRENT THROUGH JANUARY 11, 2000

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Structure search limits have been increased. See HELP SLIMIT for details.

=>

=>
=> d his l39

(FILE 'HCAPLUS' ENTERED AT 17:11:31 ON 07 OCT 2000)
SELECT HIT RN L33 1-8
SELECT HIT RN L37 1-14

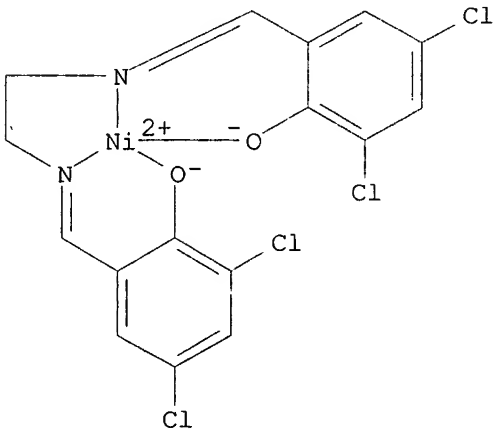
FILE 'REGISTRY' ENTERED AT 17:18:27 ON 07 OCT 2000
L39 26 S E1-E27

=> s l39 not l27

L40 26 L39 NOT L27

=> d ide can l40 1-26

L40 ANSWER 1 OF 26 REGISTRY COPYRIGHT 2000 ACS
RN **261623-86-3** REGISTRY
CN Nickel, [[2,2'-[1,2-ethanediylbis[(nitrilo-.kappa.N)methylidyne]]bis[4,6-dichlorophenolato-.kappa.O]](2-)]- (9CI) (CA INDEX NAME)
MF C16 H10 Cl4 N2 Ni O2
CI CCS
SR CA
LC STN Files: CA, CAPLUS



1 REFERENCES IN FILE CA (1967 TO DATE)
1 REFERENCES IN FILE CAPLUS (1967 TO DATE)

REFERENCE 1: 132:231088

L40 ANSWER 2 OF 26 REGISTRY COPYRIGHT 2000 ACS
RN **246047-02-9** REGISTRY
CN Nickel(1+), [[(3R)-3,4-bis[[[2-(hydroxy-.kappa.O)phenyl]methylene]amino-.kappa.N]butyl]dimethylsulfoniumato(2-)]-, (SP-4-4)- (9CI) (CA INDEX NAME)
MF C20 H23 N2 Ni O2 S

```
=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 17:19:52 ON 07 OCT 2000
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2000 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.

FILE COVERS 1967 - 7 Oct 2000  VOL 133 ISS 16
FILE LAST UPDATED: 6 Oct 2000  (20001006/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

 This file supports REG1stRY for direct browsing and searching of
 all substance data from the REGISTRY file.  Enter HELP FIRST for
 more information.

Now you can extend your author, patent assignee, patent information,
and title searches back to 1907.  The records from 1907-1966 now have
this searchable data in CAOLD.  You now have electronic access to all
of CA: 1907 to 1966 in CAOLD and 1967 to the present in HCAPLUS on STN.

=>

=>

=> d stat que l42 nos

L5              STR
L7         18360 SEA FILE=REGISTRY SSS FUL L5
L8              STR
L9          5204 SEA FILE=REGISTRY SUB=L7 SSS FUL L8
L10             STR
L11          484 SEA FILE=REGISTRY SUB=L9 SSS FUL L10
L12             STR
L14             STR
L17          988 SEA FILE=REGISTRY SSS FUL L12 AND L14
L18             STR
L19           60 SEA FILE=REGISTRY SUB=L17 SSS FUL L18
L20          418 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L11
L21           89 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L19
L23         5172 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L7
L24          895 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L17
L25            4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L23 AND L24
L27            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  DNA/CN
L28               SEL  PLU=ON  L27 1- CHEM :       4 TERMS
L29       482681 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L28
L30       544802 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L29 OR DNA OR ?DEOXYRIBONU?
L31       528726 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L30 NOT (?DNASE? OR DNASE?)
L33            8 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20 AND ?NUCLEIC?(5A)ACID
L36           14 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20 AND (?PROTEIN? OR
                 AMINO(W)ACID OR AA OR ?PEPTID?)
L37           14 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L36 NOT (L25 OR L33)
L41           46 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L21 AND (L31 OR ?NUCLEIC? OR
                 ?PROTEIN? OR AMINO(W)ACID OR AA OR ?PEPTID?)
L42           46 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L41 NOT (L25 OR L33 OR L37)


=>
```

=>

=> d ibib abs hitrn 142 1-20;d ibib hitrn 142 21-42

L42 ANSWER 1 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 2000:445668 HCAPLUS
DOCUMENT NUMBER: 133:204603
TITLE: Metalloporphyrin mediated **DNA** cleavage by a low concentration of HaeIII restriction enzyme
AUTHOR(S): Tabata, Masaaki; Nakajima, Koji; Nyarko, Elvis
CORPORATE SOURCE: Department of Chemistry, Faculty of Science and Engineering, Saga University, Saga, 840-8502, Japan
SOURCE: J. Inorg. Biochem. (2000), 78(4), 383-389
CODEN: JIBIDJ; ISSN: 0162-0134
PUBLISHER: Elsevier Science Inc.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The plasmid **DNA** scission by the restriction enzyme HaeIII was investigated in the presence of tetrakis(1-methylpyridinium-4-yl)porphyrin (H2TMPyP) and its manganese(III), iron(III), nickel(II), cobalt(III) and zinc(II) derivs. The effect of metalloporphyrins on plasmid **DNA** cleavage was ascertained by gel electrophoresis, UV-Vis absorption spectroscopy and CD spectroscopy. In the absence of the metalloporphyrins, plasmid **DNA** scission did not occur in the presence of a low concn. of HaeIII (0.2 units .mu.L-1) at 37.degree.C after 1 h incubation. However, **DNA** cleavage occurred in the presence of the metalloporphyrins and HaeIII (0.2 units .mu.L-1) at 37.degree.C after 1 h incubation. Gel electrophoresis results indicate the catalytic effect of metalloporphyrins (Mn(III)-, Fe(III)-, Co(III)- and Zn(II)TMPyP) by binding to both **DNA** and the enzyme through electrostatic interaction, which was confirmed by the change in UV-Vis and CD spectra. A mechanism for the enhanced **DNA** cleavage is proposed.
IT **48242-71-3**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BIOL (Biological study); PROC (Process)
(metalloporphyrin mediated **DNA** cleavage by a low concn. of HaeIII restriction enzyme)
REFERENCE COUNT: 20
REFERENCE(S): (1) Aggarwal, A; Curr Opin Struct Biol 1995, V5, P11 HCAPLUS
(2) Bhagwat, A; Methods Enzymol 1992, V216, P199 HCAPLUS
(3) Carvlin, M; Nucleic Acids Res 1983, V11, P6121 HCAPLUS
(4) Connolly, B; J Biochem 1984, V259, P10760 HCAPLUS
(5) Dougherty, G; Inorg Biochem 1988, V34, P95 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 2 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 2000:133485 HCAPLUS
DOCUMENT NUMBER: 132:175853
TITLE: Tetrapyrroles for treatment of amyloidogenic diseases
INVENTOR(S): Caughey, Winslow S.; Caughey, Byron
PATENT ASSIGNEE(S): United States Dept. of Health and Human Services, USA
SOURCE: PCT Int. Appl., 47 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE

WO 2000009111 A2 20000224 WO 1999-US18297 19990811
W: AE, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CR, CU, CZ, DE, DK, DM, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZA, ZW, AM, ZA, BY, KG, KZ, MD, RU, TJ, TM
RW: GH, GM, KE, LS, MW, SD, SL, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG
AU 9956730 A1 20000306 AU 1999-56730 19990811
PRIORITY APPLN. INFO.: US 1998-96148 19980811
WO 1999-US18297 19990811

OTHER SOURCE(S): MARPAT 132:175853

AB Methods, compds. and compns. are disclosed for treating amyloidogenic diseases, and particularly prion diseases assocd. with conversion of protease sensitive prion **protein** (PrP-sen) to protease resistant PrP (PrP-res), by administering therapeutically effective amts. of a tetrapyrrole. Particular disclosed tetrapyrroles having this activity include phthalocyanines, deuteroporphyrins, and meso-substituted porphines. Metal complexes of certain pyrroles are particularly effective in converting the conversion of PrP-sen to PrP-res. The compds. of the present invention are particularly suited for preventing or inhibiting the progression of prion-related diseases, such as transmissible spongiform encephalopathies. For example, treatment of scrapie in transgenic mice overexpressing the hamster PrP-sen as a model with either PCTS-Fe3+ (a tetrasulfonylphthalocyanine complex) (5 mg/kg) or DPG2-Fe3+ (a deuteroporphyrin glycol complex) (30 mg/kg) increased mean survival times by 40 and 37 days, resp. PcTS-Ni2+ and TMPP-Fe3+ (tetramesoporphyrin complex) (10 mg/kg each) have also been shown to increase survival times by a min. of 35 and 53 days, resp.

IT **48242-71-3**
RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(tetrapyrroles for treatment of amyloidogenic diseases)

L42 ANSWER 3 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 2000:69945 HCAPLUS
DOCUMENT NUMBER: 133:14152
TITLE: Meso-substituted cationic porphyrins interact with dsDNA and exhibit different localization patterns in radiation-induced fibrosarcoma cells
AUTHOR(S): Tobin, William R.; Greene, Robert S.
CORPORATE SOURCE: Department of Biological Sciences, State University of New York at Buffalo, Buffalo, NY, 14260, USA
SOURCE: Anticancer Res. (1999), 19(4B), 2953-2958
CODEN: ANTRD4; ISSN: 0250-7005
PUBLISHER: International Institute of Anticancer Research
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Meso-substituted cationic porphyrins were examd. for binding dsDNA. Subcellular localization time studies used Confocal Laser Scanning Microscopy of radiation-induced fibrosarcoma (RIF) cells incubated with porphyrins. Binding studies revealed a reversible interaction between porphyrin and dsDNA that is a function of **DNA** shape. Binding was inhibited at high salt concns., and enhanced by heat and **DNA** denaturants such as DMF. Trans dicationic porphyrin required more stringent binding conditions than cis dicationic and tetracationic porphyrins. Phenol extn. of porphyrin from the **DNA**-porphyrin complex demonstrates that cationic porphyrins do not damage dsDNA at high concns. Localization studies within a 24-h range reveal different distribution patterns. Metal chelates of tetracationic porphyrin exhibited a cytoplasmic localization with the exception of the zinc chelate. Localization of other metal chelates appears to be redistributed to lysosomes and mitochondria between 3 and 6 h post-incubation. HPPH used in PDT clin. trials localizes to the cytoplasmic compartment.

IT **48242-71-3**
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(meso-substituted cationic porphyrins interact with dsDNA and exhibit different localization patterns in fibrosarcoma cells)
REFERENCE COUNT: 26
REFERENCE(S):
(2) Berezney, R; Int Rev Cytology 1995, V162A, P1 HCAPLUS
(3) Bhawalkar, J; Scanning 1996, V18(8), P562 HCAPLUS
(4) Brown, P; Science 1979, V206, P1081 HCAPLUS
(5) Cortadas, J; Biochim Biophys Acta 1977, V476(3), P203 HCAPLUS
(8) Fiel, R; Biomolecular Structure Dynamics 1989, V6, P1259 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 4 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1998:679773 HCAPLUS
DOCUMENT NUMBER: 130:32683
TITLE: Inhibition of protease-resistant prion **protein** formation by porphyrins and phthalocyanines
AUTHOR(S): Caughey, Winslow S.; Raymond, Lynne D.; Horiuchi, Motohiro; Caughey, Byron
CORPORATE SOURCE: Laboratory of Persistent Viral Diseases, Rocky Mountain Laboratories, National Institute of Allergy and Infectious Diseases, National Institutes of Health, Hamilton, MT, 59840, USA
SOURCE: Proc. Natl. Acad. Sci. U. S. A. (1998), 95(21), 12117-12122
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English
AB A central aspect of pathogenesis in the transmissible spongiform encephalopathies or prion diseases is the conversion of normal protease-sensitive prion **protein** (PrP-sen) to the abnormal protease-resistant form, PrP-res. Here the authors identify porphyrins and phthalocyanines as inhibitors of PrP-res accumulation. The most potent of these tetrapyrroles had IC50 values of 0.5-1 .mu.M in scrapie-infected mouse neuroblastoma (ScNB) cell cultures. Inhibition was obsd. without effects on **protein** biosynthesis in general or PrP-sen biosynthesis in particular. Tetrapyrroles also inhibited PrP-res formation in a cell-free reaction composed predominantly of hamster PrP-res and PrP-sen. Inhibitors were found among phthalocyanines, deuteroporphyrins IX, and meso-substituted porphines; examples included compds. contg. anionic neutral protic, and cationic peripheral substituents and various metals. The authors conclude that certain tetrapyrroles specifically inhibit the conversion of PrP-sen to PrP-res without apparent cytotoxic effects. The inhibition obsd. in the cell-free conversion reaction suggests that the mechanism involved direct interactions of the tetrapyrrole with PrP-res and/or PrP-sen. These findings introduce a new class of inhibitors of PrP-res formation that represents a potential source of therapeutic agents for transmissible spongiform encephalopathies.
IT **48242-71-3**
RL: BAC (Biological activity or effector, except adverse); THU (Therapeutic use); BIOL (Biological study); USES (Uses)
(inhibition of protease-resistant prion **protein** formation by porphyrins and phthalocyanines in relation to structure)
REFERENCE COUNT: 51
REFERENCE(S):
(1) Akins, D; J Phys Chem 1996, V100, P5420 HCAPLUS
(2) Barbanti, P; Neurology 1996, V47, P734 HCAPLUS
(3) Bessen, R; Nature (London) 1995, V375, P698 HCAPLUS
(4) Bing, O; NeuroReport 1995, V6, P1369 HCAPLUS
(5) Bolton, D; J Virol 1991, V65, P3667 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L42 ANSWER 5 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1998:542971 HCAPLUS
DOCUMENT NUMBER: 129:170516
TITLE: Porphyrin compounds as telomerase inhibitors
INVENTOR(S): Wheelhouse, Richard T.; Hurley, Laurence H.
PATENT ASSIGNEE(S): Board of Regents, the University of Texas System, USA
SOURCE: PCT Int. Appl., 136 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9833503	A1	19980806	WO 1998-US2058	19980204
W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
AU 9866501	A1	19980825	AU 1998-66501	19980204
EP 988037	A1	20000329	EP 1998-908465	19980204
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
US 6087493	A	20000711	US 1998-18545	19980204
PRIORITY APPLN. INFO.:			US 1997-37295	19970205
			WO 1998-US2058	19980204

OTHER SOURCE(S): MARPAT 129:170516
AB The present invention has identified compds., such as 5,10,15,20-tetra(N-methyl-4-pyridiniumyl)porphine chloride and its metal complexes and related compds., with extended arom. chromophores that bind the G-quadruplex formed by the folding of single-stranded human telomeric **DNA**. These compds. are effective telomerase inhibitors and are contemplated to be useful in developing cancer treatments. A model of cationic porphyrin interaction with quadruplex **DNA** by intercalation was established and in combination with structure activity relations provided novel porphyrin compds. that exhibit discrimination between binding duplex and quadruplex **DNA** and show improved activity against telomerase. Thus, 5,10,15,20-tetra(N-ethyl-4-pyridiniumyl)porphine chloride (D1) was prepd. in 96% yield by alkylating the pyridinyl analog. D1 shows 55% telomerase inhibition under the conditions described herein.
IT **79407-86-6**
RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); THU (Therapeutic use); BIOL (Biological study); PROC (Process); USES (Uses)
(cationic porphyrin compds. as telomerase inhibitors for cancer treatment)

L42 ANSWER 6 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1998:329372 HCAPLUS
DOCUMENT NUMBER: 129:91841
TITLE: A study of metalloporphyrin-polynucleotide interactions by microcalorimetry and circular dichroism
AUTHOR(S): Wheeler, G.; Miskovsky, P.; Jancura, D.; Chinsky, L.
CORPORATE SOURCE: LPBC, Universite Paris VI, Paris, 75252, Fr.
SOURCE: J. Biomol. Struct. Dyn. (1998), 15(5), 967-985
CODEN: JBSDD6; ISSN: 0739-1102
PUBLISHER: Adenine Press
DOCUMENT TYPE: Journal

LANGUAGE: English
AB The interactions of calf thymus **DNA** and the model polynucleotides poly(dA).poly(dT), poly(dAdT)2 and poly(dG.dC)2 with a group of metalloporphyrins derived from the free base porphyrin tetrakis(4-N-methylpyridyl)porphine, H2(TMpyP4) were examd. by means of UV absorption spectroscopy, CD spectroscopy, and microcalorimetry. The interactions of the Cu, Co, Ni, and Zn derivs. of H2(TMpy-P4) in addn. to the free base porphyrin itself were studied. Strong evidence for an external self-stacking interaction of the Cu(TMpy-P4) and Zn(TMpy-P4) derivs. with poly(dA).poly(dT) and poly(dAdT)2 was found even at low concns. of porphyrin, and all of the porphyrin derivs. studied appear to display such a self-stacking in interaction with poly(dA.dT)2 at sufficiently high ratios of porphyrin to polynucleotide.
IT **48242-71-3**
RL: RCT (Reactant)
(metalloporphyrin-polynucleotide interactions)

L42 ANSWER 7 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1998:132907 HCAPLUS
DOCUMENT NUMBER: 128:254827
TITLE: Electrochemical studies of NiTMpyP and interaction with **DNA**
AUTHOR(S): Qu, Feng; Li, Nan-Qiang; Jiang, Yu-Yang
CORPORATE SOURCE: Department of Chemistry, Peking University, Beijing, 100 871, Peop. Rep. China
SOURCE: Talanta (1998), 45(5), 787-793
CODEN: TLNTA2; ISSN: 0039-9140
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English
AB In this paper, cyclic voltammetry, linear sweep voltammetry and chronocoulometry in connection with the hang mercury drop electrode were used to study NiTMpyP and its mixt. with **DNA**. The redn. of NiTMpyP in our exptl. conditions involves in 4e redn. of TMpyP. NiTMpyP interacting with **DNA** forms electrochem. non-active complex **DNA**-2NiTMpyP, which can not be reduced on the Hg electrode. The peak potential of NiTMpyP does not shift and its electrochem. kinetic parameters indicate no significant change in the presence of **DNA**. However, the redn. current of NiTMpyP decreases obviously due to the formation of **DNA**-2NiTMpyP, which implies its equil. concn. decreases when **DNA** was mixed. The decrease of peak current is proportional to **DNA** concn., which can be applied to est. **DNA** concn.
IT **48242-71-3D**, complex with **DNA**
RL: ARG (Analytical reagent use); DEV (Device component use); FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); ANST (Analytical study); FORM (Formation, nonpreparative); PROC (Process); USES (Uses)
(electrochem. studies of NiTMpyP and interaction with **DNA**)
IT **48242-71-3**
RL: PEP (Physical, engineering or chemical process); PROC (Process)
(electrochem. studies of NiTMpyP and interaction with **DNA**)

L42 ANSWER 8 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1998:2869 HCAPLUS
DOCUMENT NUMBER: 128:110460
TITLE: Comparison of metalloporphyrins interacting with **DNA**
AUTHOR(S): Qu, Feng; Li, Nan Qiang
CORPORATE SOURCE: Department Chemistry, Peking University, Beijing, 100871, Peop. Rep. China
SOURCE: Electroanalysis (1997), 9(17), 1348-1352
CODEN: ELANEU; ISSN: 1040-0397
PUBLISHER: Wiley-VCH Verlag GmbH
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of metalloporphyrins (CuTMpyP, CuTMAP, CuTPPS, NiTMpyP, ZnTMpyP, and CdTMpyP) reacting with **DNA** were compared. The interaction of metalloporphyrin with **DNA** shows different binding modes and electrochem. behavior when either the metal ion or porphyrin ligand is different. Due to electrostatical repulsion, interaction between the anionic substitute group and a phosphate group on **DNA** mol. backbone, it is difficult for the anionic porphyrin to interact with **DNA**. The ability of cationic porphyrins to react with **DNA** depends on the size of the substitute group and the metal ion in the porphyrin plane center. Metalloporphyrin with or without axial ligand, which depends on the metal ion, results in outside binding or intercalating modes, and shows different interaction capability with **DNA**. The conditional binding consts. of NiTMpyP, CuTMpyP, and CuTMAP, which mainly show intercalating mode to **DNA**, were evaluated.

IT **48242-71-3P**
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(metalloporphyrins interacting with **DNA** as model for antitumor agents)

L42 ANSWER 9 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1997:725559 HCAPLUS
DOCUMENT NUMBER: 128:11168
TITLE: Role of the porphyrin excited states in their interactions with **DNA** and **DNA** - model compounds in aqueous solutions
AUTHOR(S): Galievsky, V.; Chirvony, V.; Ermolenkov, V.; Kruglik, S.; Mojzes, P.; Turpin, P. -Y.
CORPORATE SOURCE: Institute of Molecular and Atomic Physics, Acad. Sci. Belarus, Minsk, BY-220072, Belarus
SOURCE: Spectrosc. Biol. Mol.: Mod. Trends, [Eur. Conf.], 7th (1997), 351-354. Editor(s): Carmona, Pedro; Navarro, Raquel; Hernanz, Antonio. Kluwer: Dordrecht, Neth. CODEN: 65FQAE
DOCUMENT TYPE: Conference; General Review
LANGUAGE: English

AB A review with 13 refs. The authors focus on the photophysics and excited state dynamics of the Cu(II)- and Ni(II)- derivs. of H2(TMpy-P4), which are in their ground state 4 coordinate and a mixt. of 4- and 6 coordinate species, resp., and thus able to undergo various kinds of photoinduced axial water ligation/release processes on the one hand, and two main types of binding to **DNA**, i.e. outside or groove-binding and intercalation between base pairs, on the other.

IT **48242-71-3**
RL: BPR (Biological process); PRP (Properties); BIOL (Biological study); PROC (Process)
(role of porphyrin excited states in interactions with **DNA** and **DNA** - model compds. in aq. solns.)

L42 ANSWER 10 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1997:583267 HCAPLUS
DOCUMENT NUMBER: 127:272360
TITLE: A UV resonant Raman spectroscopic study of the interaction of metallic derivatives of Tetrakis(4-N-methylpyridyl)porphine with polynucleotides
AUTHOR(S): Wheeler, G. V.; Laigle, A.; Chinsky, L.
CORPORATE SOURCE: Equipe ESTER, L.P.B.C. (CNRS URA 2056), Case 138, Universite Pierre et Marie Curie, Paris, 75252, Fr.
SOURCE: J. Biomol. Struct. Dyn. (1997), 15(1), 107-117 CODEN: JBSDD6; ISSN: 0739-1102
PUBLISHER: Adenine Press
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Resonance Raman spectra excited at 257 nm are reported for the complexes of the Nickel, Cobalt and Zinc derivs. of Tetrakis(4-N-methylpyridyl)porphine with poly(dA.dT)2, poly(dA).poly(dT), poly(dG.dC)2 and poly(dG).poly(dC). These spectra are interpreted as evidence of multiple outside binding modes with poly(dA).poly(dT), and of evidence for an outside binding mode with Poly(dG.dC)2. Some results obtained for the zinc deriv. with poly(dA).poly(dT) suggest a binding mode peculiar to this deriv.

IT **48242-71-3**
RL: BAC (Biological activity or effector, except adverse); PRP (Properties); BIOL (Biological study)
(interaction of metal porphyrin derivs. with polynucleotides)

L42 ANSWER 11 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1996:393976 HCAPLUS
DOCUMENT NUMBER: 125:51675
TITLE: Excited States of Water-Soluble Metal Porphyrins as Microenvironmental Probes for **DNA** and **DNA**-Model Compounds: Time-Resolved Transient Absorption and Resonance Raman Studies of Ni(TMpy-P4) in [Poly(dG-dC)]2 and [Poly(dA-dT)]2
AUTHOR(S): Galievsky, Victor A.; Chirvony, Vladimir S.; Kruglik, Sergei G.; Ermolenkov, Vladimir V.; Orlovich, Valentine A.; Otto, Cees; Mojzes, Peter; Turpin, Pierre-Yves
CORPORATE SOURCE: Institute of Molecular and Atomic Physics, Minsk, 220072, Belarus
SOURCE: J. Phys. Chem. (1996), 100(30), 12649-12659
CODEN: JPCHAX; ISSN: 0022-3654
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The dynamics and mechanisms of photoexcitation relaxation of the water-sol. cationic metalloporphyrin nickel(II) 5,10,15,20-tetrakis[4-(N-methylpyridyl)] porphyrin (Ni(TMpy-P4)) bound to **DNA**-model polynucleotides, i.e. poly(dG-dC)2 and poly(dA-dT)2, and free in a mere phosphate buffer, have been studied in detail by using time-resolved picosecond transient absorption (TA) and nanosecond resonance Raman (RR) spectroscopies. For the Ni(TMpy-P4)-poly(dG-dC)2 complex, double-exponential kinetics of relaxation has been found, with time consts. of .ltoreq.10 and 350.+-.20 ps, and abs. absorption spectra have been reconstructed from exptl. measured difference spectra. The long-lived transient species has been assigned to the excited intramol. metal-centered (d,d) state 3B1g of the 4-coordinate Ni porphyrin intercalated between G-C base pairs. Transient RR spectra originating from this state have also been obtained and discussed. A much more complicated process of excitation relaxation has been found for the Ni(TMpy-P4)-poly(dA-dT)2 complex, where at least four relaxation components can be sepd. with time consts. of .ltoreq.10, .apprx.100, .apprx.450, and .mchgt.1 ns. Our studies support the existence of at least two types of Ni(TMpy-P4) interaction with poly(dA-dT)2, each having its own kinetics of TA decay and transient RR spectra. Both TA and RR sets of data show that a major part of Ni porphyrin mols. yields a photophys. behavior typical for a 4-coordinate species, the excited (d,d) state 3B1g playing the key role in relaxation processes, while a minor part of Ni(TMpy-P4) also participates in axial ligand binding/release photoprocesses. Comparative anal. of transient RR spectra of Ni(TMpy-P4) bound to the A-T sequence and free in a phosphate buffer shows that no 6-coordinate 3B1g(L)2 transient species is photogenerated in the complex with poly(dA-dT)2, and therefore, axial coordination of only one extra-ligand mol. (most probably from the surrounding water soln.) to the porphyrin central Ni ion is proposed to explain the exptl. results. Possible processes of Ni(TMpy-P4) binding to poly(dA-dT)2 are discussed on the basis of the current photophys. data.

IT **48242-71-3**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)

(excited states of water-sol. metal porphyrins as microenvironmental probes for **DNA** and **DNA**-model compds. from time-resolved transient absorption and resonance Raman studies of Ni(TMpy-P4) in [poly(dG-dC)]2 and [poly(dA-dT)]2)

L42 ANSWER 12 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1996:32296 HCAPLUS
DOCUMENT NUMBER: 124:110006
TITLE: Interaction of electronically excited copper-porphyrin with **DNA** studied by resonance Raman spectroscopy
AUTHOR(S): Lu, Dongsheng; Lu, Lin; Zhao, Xiaojie; An, Chengwu; Fan, Yongchang; Jiang, Shan; Li, Zaiguang; Huang, Suqiu
CORPORATE SOURCE: State Key Laboratory of laser Technology, Huazhong University of Science and Technology, Wuhan, 430074, Peop. Rep. China
SOURCE: Chin. Sci. Bull. (1995), Volume Date 1995, 40(18), 1552-7
CODEN: CSBUEF; ISSN: 1001-6538
DOCUMENT TYPE: Journal
LANGUAGE: English
AB This note, the interactions of three kinds of new porphyrin Cu (NACN) [Cu-tetrakis (4-N-acetonitrile pyridyl) porphine], Cu (NEAE) and Ni(NEAE) [Cu- and Ni-tetrakis (4N-ethylacetate pyridyl) porphine] with **DNA** are studied by resonance Raman spectroscopy, and the mechanisms of exciplex formation are discussed.
IT **127878-73-3**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(interaction of electronically excited copper-porphyrin with **DNA** studied by resonance Raman spectroscopy)

L42 ANSWER 13 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1995:979946 HCAPLUS
DOCUMENT NUMBER: 124:109992
TITLE: Resonance Raman and transient absorption studies on Ni(TMpy-P4) in a water buffer and bound to **DNA** model compounds: Excited-states dynamics and state of coordination.
AUTHOR(S): Ermolenkov, V. V.; Kruglik, S. G.; Orlovich, V. A.; Chirvony, V. S.; Galievsky, V. A.; Mojzes, P.; Chinsky, L.; Turpin, P. -Y.
CORPORATE SOURCE: B.I.Stepanov Institute Physics, Academy Sciences Belarus, Minsk, 220072, Belarus
SOURCE: Spectrosc. Biol. Mol., Eur. Conf., 6th (1995), 221-2. Editor(s): Merlin, Jean Claude; Turrell, Sylvia; Huvenne, Jean Pierre. Kluwer: Dordrecht, Neth.
CODEN: 62BKAN
DOCUMENT TYPE: Conference
LANGUAGE: English
AB Nanosecond resonance Raman spectra (RR) of water-sol. Ni(TMpy-P4) bound to **DNA** model compds. poly(dA-dT) and poly(dG-dC) show prominent transient features under increasing power d. of the excitation pulses. Careful comparison with RR spectra of four- and six-coordinate Ni(TMpy-P4) in water buffer, as well as of the related Ni(II)-porphyrin, Ni-TPP, in both non-coordinating (benzene) and coordinating N-contg. solvents, revealed that it is the low-lying excited (d,d) state of Ni(TMpy-P4) that manifests itself in RR spectra under increasing excitation power d. The results of picosecond transient absorption studies on the kinetics and relaxation pathways for Ni(TMpy-P4) in different mol. environments are also presented. Although transient RR spectra of Ni(TMpy-P4) in both poly(dA-dT) and poly(dG-dC) reveal similar peculiarities, application of the picosecond absorption technique permits distinction between the photophysics, depending on the type of Ni-porphyrin complexation with the polynucleotides, with more complex behavior for Ni(TMpy-P4) in

poly(dA-dT).

IT **48242-71-3**
RL: BPR (Biological process); PRP (Properties); BIOL (Biological study); PROC (Process)
(resonance Raman and transient absorption studies of excited-state dynamics and coordination of Ni(TMpy-P4) in aq. buffer and bound to **DNA** model compds.)

L42 ANSWER 14 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1995:979940 HCAPLUS
DOCUMENT NUMBER: 124:109989
TITLE: Time-resolved resonance Raman and transient absorption studies on the excited states of metalloporphyrins and metalloporphyrin-**DNA** interactions
AUTHOR(S): Kruglik, S. G.; Apanasevich, P. A.; Chirvony, V. S.; Orlovich, V. A.; Turpin, P. -Y.
CORPORATE SOURCE: B.I.Stepanov Institute Physics, Academy Sciences Belarus, Minsk, 220072, Belarus
SOURCE: Spectrosc. Biol. Mol., Eur. Conf., 6th (1995), 207-10. Editor(s): Merlin, Jean Claude; Turrell, Sylvia; Huvenne, Jean Pierre. Kluwer: Dordrecht, Neth. CODEN: 62BKAN
DOCUMENT TYPE: Conference
LANGUAGE: English
AB The Cu(II)- and Ni(II)-derivs. of water-sol. H2-5,10,15,20-tetrakis[4-(N-methylpyridyl)]porphyrin and their complexes with **DNA** model polynucleotides poly(dA-dT)2 and poly(dG-dC)2 were investigated by time-resolved resonance Raman and transient absorption spectroscopies. The dynamics of the exciplex formation/decay and origin of its excited state were examd.
IT **48242-71-3 48242-71-3D, DNA** complexes
RL: PEP (Physical, engineering or chemical process); PRP (Properties); PROC (Process)
(time-resolved resonance Raman and transient absorption studies on the excited states of metalloporphyrins and metalloporphyrin-**DNA** interactions)

L42 ANSWER 15 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1995:930483 HCAPLUS
DOCUMENT NUMBER: 124:100852
TITLE: SERRS of new copper and nickel porphyrins and effect of **DNA**
AUTHOR(S): Zhou, Guang-Ming; Sheng, Rong-Sheng; Xiong, Ya; Xu, Zhi-San; Wang, Xiao-Hua; Zeng, Yun-E.
CORPORATE SOURCE: Center of Analysis and Measurement, Wuhan University, Wuhan, 430072, Peop. Rep. China
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (1995), 16(10), 1541-3 CODEN: KTHPDM; ISSN: 0251-0790
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB The SERRS spectra of Cu and Ni complexes of meso-tetrakis(4-N-ethoxycarbonylmethylpyridyl)porphyrin on Ag sols and the effect of calf thymus double strand **DNA** were studied. The SERRS bands assignments are given.
IT **127878-73-3 127878-73-3D, DNA** complex
RL: PRP (Properties)
(surface-enhanced resonance Raman spectra of)

L42 ANSWER 16 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1995:927238 HCAPLUS
DOCUMENT NUMBER: 123:332983
TITLE: Study of the interaction of water-soluble metalloporphyrins with **DNA** by microcalorimetry
AUTHOR(S): Xiong, Ya; Huang, Suqiu; Wu, Dingquan; Qu, Songsheng
CORPORATE SOURCE: Dep. Chem., Wuhan Univ., Wuhan, 430072, Peop. Rep.

China
SOURCE: Wuli Huaxue Xuebao (1995), 11(10), 957-60
CODEN: WHXUEU; ISSN: 1000-6818
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB The interactions of water-sol. metalloporphyrins, Cu(NACN) [Cu-tetrakis(4-N-acetonitrilepyridyl)porphyrin] and Ni(NEAE) [Ni-tetrakis(4-N-ethylacetatepyridyl)porphyrin], with calf thymus double-stranded (ds)**DNA** and single-stranded (ss)**DNA** were investigated by microcalorimetry and UV spectroscopy. The results demonstrated that the reaction of Cu(NACN) with dsDNA was endothermic with a binding enthalpy (.DELTA.H) of 9.2 kJ/mol for Cu(NACN) with a satd. binding no. of 4-5 base pairs (bp) and that the reaction of Ni(NEAE) with dsDNA was exothermic with .DELTA.H = 7.6 kJ/mol and a satd. binding no. of 5-6 bp. The difference in their binding modes were mainly due to the metal ionic properties in porphyrin mols. The water-sol. porphyrins, Cu(NECN) and Ni(NEAE), interacted with ssDNA more intensively.
IT **127878-73-3**
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(thermodn. of interaction of water-sol. metalloporphyrins with **DNA**)

L42 ANSWER 17 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1995:691462 HCAPLUS
DOCUMENT NUMBER: 123:105501
TITLE: Perturbations in **DNA** structure upon interaction with porphyrins revealed by chemical probes, **DNA** footprinting and molecular modeling
AUTHOR(S): Ford, Kevin G.; Neidle, Stephen
CORPORATE SOURCE: Institute Cancer Research, CRC Biomolecular Structure Unit, Surrey, SM2 5NG, UK
SOURCE: Bioorg. Med. Chem. (1995), 3(6), 671-7
CODEN: BMECEP; ISSN: 0968-0896
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The interactions of several porphyrins with a 74 base-pair **DNA** sequence have been examd. by footprinting and chem. protection methods. Tetra-(4-N-methyl-(pyridyl)) porphyrin (TMPy), two of its metal complexes (with Ni or Pd) and tetra-(4-trimethylanilinium) porphyrin (TMAP) bind to closely similar AT-rich sequences. The three TMPy ligands produce modest changes in **DNA** structure and base accessibility on binding, in contrast to the large-scale conformational changes obsd. with TMAP. Mol. modeling studies have been performed on TMPy and TMAP bound in the AT-rich minor groove of an oligonucleotide. These have shown that significant structural change is needed to accommodate the bulky tri-Me substituent groups of TMAP, in contrast to the facile minor groove fit of TMPy.
IT **79407-86-6**
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(perturbations in **DNA** structure upon interaction with porphyrins)

L42 ANSWER 18 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1995:51810 HCAPLUS
DOCUMENT NUMBER: 122:100030
TITLE: Studies of interaction of electronically excited water-soluble copper-porphyrins with **DNA** by resonance Raman spectroscopy
AUTHOR(S): Zhao, Xiao-Jie; Jiang, Shan; Lu, Dong-Sheng; Lu, Lin; Mao, Ci-Bo; An, Cheng-Wu; Fan, Yong-Chang; Li, Zai-Guang; Zhou, Xiang; Huang, Su-Qiu
CORPORATE SOURCE: Natl. Lab. Laser Technol., Huazhong Univ. Sci. Technol., Wuhan, 430074, Peop. Rep. China
SOURCE: Gaodeng Xuexiao Huaxue Xuebao (1994), 15(4), 600-2
CODEN: KTHPDM; ISSN: 0251-0790
DOCUMENT TYPE: Journal

LANGUAGE: Chinese
AB The resonance Raman spectra of water-sol. porphyrin Cu(NACN) [Cu-tetrakis(4-N-acetonitrilepyridyl)porphyrin], Cu(NEAE) and Ni(NEAE) [Cu or Ni-tetrakis(4-N-ethylacetatepyridyl)porphyrin] and their complexes with calf thymus **DNA** at different laser pulse powers were measured with 445 nm pulse laser excitation. The anal. results indicate that both of the copper-porphyrins formed electronic exciplex with **DNA** but the Ni(NEAE) did not form. In this expt., besides copper-porphyrin Raman bands VI (near 1370 cm-1) and VIII (near 1570 cm-1), band VII (near 1470 cm-1) also show extra band which symbolizes the formation of exciplex. The triplet of copper-porphyrin with a long life time quenched by **DNA** and the exciplex may be formed by charge transfer from triplet of Cu-porphyrin to **DNA**.
IT **127878-73-3**
RL: BPR (Biological process); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process)
(interaction of electronically excited water-sol. copper-porphyrins and nickel-porphyrin with **DNA**)

L42 ANSWER 19 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1995:26895 HCAPLUS
DOCUMENT NUMBER: 122:3755
TITLE: The interaction of water-soluble quaternary ammonium pyridine porphyrins with **DNA** studied by resonance Raman spectroscopy
AUTHOR(S): Zhao, Xiao-jie; Jiang, Shan; Lu, Dong-sheng; Huang, Su-qiu; Li, Zai-guang
CORPORATE SOURCE: Natl. Lab. Laser Technol., Huazhong Univ. Sci. and Tech., Wuhan, 430074, Peop. Rep. China
SOURCE: Shengwu Huaxue Zazhi (1994), 10(3), 308-12
CODEN: SHZAE4; ISSN: 1000-8543
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB The interaction of metal water-sol. porphyrins Cu(NEAE), Ni(NEAE) [Cu or Ni-tetrakis (4-N-ethylacetatepyridyl) Porphine] and Cu(NACN) [Cu-tetrakis (4-N-acetonitrilepyridyl) Porphine] with calf thymus **DNA** has been investigated by resonance Raman and UV-visible spectroscopy. The results demonstrated that Cu(NEAE), Ni(NEAE) and Cu(NACN) interact with **DNA** by outside-binding, partial intercalation and groove-binding resp.; the intercalated structure requires the rotation of the pyridyl rings toward the porphyrin core plane, but it is impossible to rotate co-plane with porphyrin core plane. The pyridyl rings may rotate toward perpendicular direction or co-plane direction with porphyrin core plane for non-intercalated structure. The size and steric hindrance of substituent of porphyrin is one of the crucial factors to affect the interaction between porphyrins and **DNA**.
IT **127878-73-3**
RL: PRP (Properties)
(**DNA** partial intercalation of)

L42 ANSWER 20 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1994:48297 HCAPLUS
DOCUMENT NUMBER: 120:48297
TITLE: Sequence specific interaction of **DNA** with water-soluble porphyrins
AUTHOR(S): Kuroda, Reiko; Tanaka, Hajime; Watanabe, Satoru
CORPORATE SOURCE: Coll. Arts Sci., Univ. Tokyo, Tokyo, 153, Japan
SOURCE: Nucleic Acids Symp. Ser. (1993), 29(Second International Symposium on Nucleic Acids Chemistry), 123-4
CODEN: NACSD8; ISSN: 0261-3166
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Footprinting expts. and restriction enzyme inhibition work as well as affinity cleavage studies have been carried out to probe the sequence specific recognition of **DNA** by water-sol. free-base porphyrins

and their metal complexes. Porphyrins lacking functional groups capable of forming hydrogen bonds exhibited high **DNA** sequence specificity. Induced CD spectroscopy was found useful in analyzing the complex **DNA** binding modes of these compds.

IT **48242-71-3 128246-76-4**
RL: PRP (Properties)
(**DNA** binding mode of)

L42 ANSWER 21 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1993:530904 HCAPLUS
DOCUMENT NUMBER: 119:130904
TITLE: The search for structure-specific **nucleic** acid-interactive drugs: Effects of compound structure on RNA versus **DNA** interaction strength
AUTHOR(S): Wilson, W. David; Ratmeyer, Lynda; Zhao, Min; Strekowski, Lucjan; Boykin, David
CORPORATE SOURCE: Dep. Chem., Georgia State Univ., Atlanta, GA, 30303, USA
SOURCE: Biochemistry (1993), 32(15), 4098-104
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **48242-71-3**, Ni-P 4
RL: BIOL (Biological study)
(RNA binding by, structure effect on, antiviral design in relation to)

L42 ANSWER 22 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1991:508741 HCAPLUS
DOCUMENT NUMBER: 115:108741
TITLE: Long-range fluorescence quenching of ethidium ion by cationic porphyrins in the presence of **DNA**
AUTHOR(S): Pasternack, Robert F.; Caccam, Melissa; Keogh, Bart; Stephenson, Thomas A.; Williams, Alison P.; Gibbs, Esther J.
CORPORATE SOURCE: Dep. Chem., Swarthmore Coll., Swarthmore, PA, 19081, USA
SOURCE: J. Am. Chem. Soc. (1991), 113(18), 6835-40
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **48242-71-3**
RL: BIOL (Biological study)
(**DNA**-ethidium complex fluorescence quenching by, mechanism of)

L42 ANSWER 23 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1991:467085 HCAPLUS
DOCUMENT NUMBER: 115:67085
TITLE: Nickel(II) porphyrin binding to anionic biopolymers investigated by resonance Raman and optical spectroscopy
AUTHOR(S): Yue, K. T.; Lin, Mengfen; Gray, Thomas A.; Marzilli, Luigi G.
CORPORATE SOURCE: Dep. Chem., Emory Univ., Atlanta, GA, 30322, USA
SOURCE: Inorg. Chem. (1991), 30(16), 3214-22
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **48242-71-3 128235-51-8**
RL: BIOL (Biological study)
(structure and coordination properties of, **nucleic** acids and other anionic biopolymers binding effect on)

L42 ANSWER 24 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1991:429823 HCAPLUS
DOCUMENT NUMBER: 115:29823
TITLE: Effect of N-alkyl substituents on the **DNA** binding properties of meso-tetrakis(4-N-alkylpyridinium-4-yl)porphyrins and their nickel derivatives
AUTHOR(S): Gray, Thomas A.; Yue, Kwok To; Marzilli, Luigi G.
CORPORATE SOURCE: Dep. Chem., Emory Univ., Atlanta, GA, 30322, USA
SOURCE: J. Inorg. Biochem. (1991), 41(3), 205-19
CODEN: JIBIDJ; ISSN: 0162-0134
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **79407-86-6 133288-46-7 133288-47-8**
RL: RCT (Reactant)
(effect of N-alkyl substituents on the **DNA** binding properties of)

L42 ANSWER 25 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1990:606873 HCAPLUS
DOCUMENT NUMBER: 113:206873
TITLE: Interactions of porphyrins and metalloporphyrins with single-stranded poly(dA)
AUTHOR(S): Pasternack, R. F.; Brigandi, R. A.; Abrams, M. J.; Williams, A. P.; Gibbs, E. J.
CORPORATE SOURCE: Dep. Chem., Swarthmore Coll., Swarthmore, PA, 19081, USA
SOURCE: Inorg. Chem. (1990), 29(22), 4483-6
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **48242-71-3**
RL: BIOL (Biological study)
(poly(deoxyriboadenylate) interaction with)

L42 ANSWER 26 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1990:454512 HCAPLUS
DOCUMENT NUMBER: 113:54512
TITLE: Interaction of water-soluble copper(II), nickel(II), and cobalt(III) porphyrins with polynucleotides
AUTHOR(S): Butje, Kai; Nakamoto, Kazuo
CORPORATE SOURCE: Dep. Chem., Marquette Univ., Milwaukee, WI, 53233, USA
SOURCE: J. Inorg. Biochem. (1990), 39(1), 75-92
CODEN: JIBIDJ; ISSN: 0162-0134
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **128235-51-8 128246-78-6**
RL: BIOL (Biological study)
(**DNA** and **polydeoxyribonucleotides** interaction with water-sol.)

L42 ANSWER 27 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1990:436593 HCAPLUS
DOCUMENT NUMBER: 113:36593
TITLE: IR and Raman spectroscopic studies on coulombic interaction between water-soluble porphyrins and **nucleic** acids
AUTHOR(S): Nonaka, Y.; Lu, D. S.; Dwivedi, A.; Strommen, D. P.; Nakamoto, K.
CORPORATE SOURCE: Dep. Chem., Marquette Univ., Milwaukee, WI, 53233, USA
SOURCE: Biopolymers (1990), 29(6-7), 999-1004
CODEN: BIPMAA; ISSN: 0006-3525
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **48242-71-3**
RL: BIOL (Biological study)

(**DNA** coulombic interaction with, IR and Raman spectroscopy for study of)

L42 ANSWER 28 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1990:419628 HCAPLUS
Correction of: 1990:72427
DOCUMENT NUMBER: 113:19628
Correction of: 112:72427
TITLE: Drug binding by branched **DNA**: selective interaction of tetrapyridyl porphyrins with an immobile junction
AUTHOR(S): Lu, Min; Guo, Qiu; Pasternack, Robert F.; Wink, Donald J.; Seeman, Nadrian C.; Kallenbach, Neville R.
CORPORATE SOURCE: Dep. Chem., New York Univ., New York, NY, 10003, USA
SOURCE: Biochemistry (1990), 29(6), 1614-24
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **48242-71-3**
RL: BIOL (Biological study)
(branched **DNA** binding by, characterization of)

L42 ANSWER 29 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1990:72427 HCAPLUS
DOCUMENT NUMBER: 112:72427
TITLE: Drug binding by branched **DNA**: selective interaction of tetrapyridyl porphyrins with an immobile junction
AUTHOR(S): Lu, Min; Guo, Qin; Pasternack, Robert F.; Wink, Donald J.; Seeman, Nadrian C.; Kallenbach, Neville R.
CORPORATE SOURCE: Dep. Chem., New York Univ., New York, NY, 10003, USA
SOURCE: Biochemistry (1990), 29(6), 1614-24
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **48242-71-3**
RL: BIOL (Biological study)
(branched **DNA** binding by, characterization of)

L42 ANSWER 30 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1990:50922 HCAPLUS
DOCUMENT NUMBER: 112:50922
TITLE: Interactions of water-soluble porphyrins with **hexadeoxyribonucleotides**: resonance Raman, UV-visible and proton NMR studies
AUTHOR(S): Butje, Kai; Schneider, Jinghua H.; Kim, Jung Ja P.; Wang, Yusen; Ikuta, Satoshi; Nakamoto, Kazuo
CORPORATE SOURCE: Dep. Chem., Marquette Univ., Milwaukee, WI, 53233, USA
SOURCE: J. Inorg. Biochem. (1989), 37(2), 119-34
CODEN: JIBIDJ; ISSN: 0162-0134
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **48242-71-3**
RL: BIOL (Biological study)
(**DNA** hexamer duplexes intercalation by and other interactions with, spectroscopic study of)

L42 ANSWER 31 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1989:627375 HCAPLUS
DOCUMENT NUMBER: 111:227375
TITLE: Metalloporphyrin **DNA** interactions: insights from NMR studies of **oligodeoxyribonucleotides**
AUTHOR(S): Strickland, James A.; Marzilli, Luigi G.; Wilson, W. David; Zon, Gerald
CORPORATE SOURCE: Dep. Chem., Emory Univ., Atlanta, GA, 30322, USA
SOURCE: Inorg. Chem. (1989), 28(23), 4191-8

CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **48242-71-3**
RL: BIOL (Biological study)
(**oligodeoxyribonucleotides** interaction with)

L42 ANSWER 32 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1989:53126 HCAPLUS
DOCUMENT NUMBER: 110:53126
TITLE: Interactions of water-soluble metalloporphyrins with **nucleic** acids studied by resonance Raman spectroscopy
AUTHOR(S): Schneider, Jinghua H.; Odo, Junichi; Nakamoto, Kazuo
CORPORATE SOURCE: Marquette Univ., Milwaukee, WI, 53233, USA
SOURCE: Nucleic Acids Res. (1988), 16(21), 10323-38
CODEN: NARHAD; ISSN: 0305-1048
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **48242-71-3**
RL: BIOL (Biological study)
(**DNA** interactions with, resonance Raman spectra in relation to)

L42 ANSWER 33 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1988:624941 HCAPLUS
DOCUMENT NUMBER: 109:224941
TITLE: Porphyrin and metalloporphyrin binding to **DNA** polymers: rate and equilibrium binding studies
AUTHOR(S): Strickland, James A.; Marzilli, Luigi G.; Gay, K. Michael; Wilson, W. David
CORPORATE SOURCE: Dep. Chem., Emory Univ., Atlanta, GA, 30322, USA
SOURCE: Biochemistry (1988), 27(24), 8870-8
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **48242-71-3**
RL: PROC (Process)
(**DNA** model compd. binding of)

L42 ANSWER 34 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1988:145615 HCAPLUS
DOCUMENT NUMBER: 108:145615
TITLE: Interactions of porphyrins with purified **DNA** and more highly organized structures
AUTHOR(S): Gibbs, Esther J.; Maurer, Muriel C.; Zhang, J. H.; Reiff, William M.; Hill, David T.; Malicka-Blaszkiewicz, Maria; McKinnie, Russell E.; Liu, H. Q.; Pasternack, Robert F.
CORPORATE SOURCE: Dep. Chem., Goucher Coll., Towson, MD, 21204, USA
SOURCE: J. Inorg. Biochem. (1988), 32(1), 39-65
CODEN: JIBIDJ; ISSN: 0162-0134
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **48242-71-3**
RL: BIOL (Biological study)
(**DNA** interaction with)

L42 ANSWER 35 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1987:546942 HCAPLUS
DOCUMENT NUMBER: 107:146942
TITLE: Metalloporphyrin effects on properties of **DNA** polymers
AUTHOR(S): Strickland, James A.; Banville, Debra L.; Wilson, W. David; Marzilli, Luigi G.
CORPORATE SOURCE: Dep. Chem., Emory Univ., Atlanta, GA, 30322, USA

SOURCE: Inorg. Chem. (1987), 26(20), 3398-406
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **79407-86-6 110314-04-0**
RL: PRP (Properties)
(interaction of, with **DNA**)

L42 ANSWER 36 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1987:209628 HCAPLUS
DOCUMENT NUMBER: 106:209628
TITLE: DNA sequence preferences for an intercalating porphyrin compound revealed by footprinting
AUTHOR(S): Ford, Kevin; Fox, Keith R.; Neidle, Stephen; Warning, Michael J.
CORPORATE SOURCE: CRN Biomol. Struct. Unit, Inst. Cancer Res., Sutton/Surrey, SM2 5PX, UK
SOURCE: Nucleic Acids Res. (1987), 15(5), 2221-34
CODEN: NARHAD; ISSN: 0305-1048
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **48242-71-3**
RL: BIOL (Biological study)
(DNA sequence for intercalation by)

L42 ANSWER 37 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1987:176524 HCAPLUS
DOCUMENT NUMBER: 106:176524
TITLE: Resonance Raman studies of metal tetrakis(N-methylpyridinium)porphyrin - assignments, structure sensitive lines and species equilibria
AUTHOR(S): Blom, N.; Strommen, D. P.; Nakamoto, K.
CORPORATE SOURCE: Chem. Dep., Marquette Univ., Milwaukee, WI, 53233, USA
SOURCE: Spectrosc. Biol. Mol., Proc. Eur. Conf., 1st (1985), 363-6. Editor(s): Alix, Alain J. P.; Bernard, Lucien; Manfait, Michel. Wiley: Chichester, UK.
CODEN: 55IEAG
DOCUMENT TYPE: Conference
LANGUAGE: English
IT **48242-71-3**
RL: PRP (Properties)
(Raman spectra of, **DNA** binding effect on)

L42 ANSWER 38 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1987:115819 HCAPLUS
DOCUMENT NUMBER: 106:115819
TITLE: Photocleavage of **DNA** in the presence of synthetic water-soluble porphyrins
AUTHOR(S): Praseuth, Daniele; Gaudemer, Alain; Verlhac, Jean Baptiste; Kraljic, I.; Sissoeff, I.; Guille, E.
CORPORATE SOURCE: Lab. Chim. Coord. Bioorg., Univ. Paris-Sud, Orsay, 91 405, Fr.
SOURCE: Photochem. Photobiol. (1986), 44(6), 717-24
CODEN: PHCBAP; ISSN: 0031-8655
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **48242-71-3**
RL: BIOL (Biological study)
(**DNA** photocleavage induction by)

L42 ANSWER 39 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1986:622044 HCAPLUS
DOCUMENT NUMBER: 105:222044
TITLE: Circular differential scattering and circular differential absorption of **DNA-protein** condensates and of dyes bound to

DNA-protein condensates
AUTHOR(S): Phillips, Cynthia L.; Mickols, William; Maestre, Marcos F.; Tinoco, Ignacio, Jr.
CORPORATE SOURCE: Lawrence Berkeley Lab., Univ. California, Berkeley, CA, 94720, USA
SOURCE: Biochemistry (1986), 25(24), 7803-11
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **48242-71-3D**, complexes with **DNA-protein** condensates
RL: ANST (Analytical study)
(CD of, circular differential scattering and absorption in relation to)

L42 ANSWER 40 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1986:618419 HCAPLUS
DOCUMENT NUMBER: 105:218419
TITLE: DNA binding specificity of a series of cationic metalloporphyrin complexes
AUTHOR(S): Ward, Brian; Skorobogaty, Andrew; Dabrowiak, James C.
CORPORATE SOURCE: Dep. Chem., Syracuse Univ., Syracuse, NY, 13244-1200, USA
SOURCE: Biochemistry (1986), 25(24), 7827-33
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **48242-71-3D**, DNA adducts
RL: BIOL (Biological study)
(nucleotide sequence binding specificity in)

L42 ANSWER 41 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1986:414440 HCAPLUS
DOCUMENT NUMBER: 105:14440
TITLE: Resonance Raman studies of metal tetrakis(4-N-methylpyridyl)porphine: band assignments, structure-sensitive bands, and species equilibria
AUTHOR(S): Blom, Nils; Odo, Junichi; Nakamoto, Kazuo; Strommen, Dennis P.
CORPORATE SOURCE: Chem. Dep., Marquette Univ., Milwaukee, WI, 53233, USA
SOURCE: J. Phys. Chem. (1986), 90(13), 2847-52
CODEN: JPCHAX; ISSN: 0022-3654
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **48242-71-3**
RL: RCT (Reactant)
(resonance Raman spectra in coordination of)

L42 ANSWER 42 OF 46 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1986:2342 HCAPLUS
DOCUMENT NUMBER: 104:2342
TITLE: Molecular complexes of nucleosides and nucleotides with a monomeric cationic porphyrin and some of its metal derivatives
AUTHOR(S): Pasternack, R. F.; Gibbs, E. J.; Antebi, A.; Bassner, S.; De Poy, L.; Turner, D. H.; Williams, A.; Laplace, F.; Lansard, M. H.; et al.
CORPORATE SOURCE: Dep. Chem., Swarthmore Coll., Swarthmore, PA, 19081, USA
SOURCE: J. Am. Chem. Soc. (1985), 107(26), 8179-86
CODEN: JACSAT; ISSN: 0002-7863
DOCUMENT TYPE: Journal
LANGUAGE: English
IT **48242-71-3D**, nucleoside and nucleotide complexes
RL: PRP (Properties)
(properties of, **DNA**-porphyrin interactions in relation to)

```
=> fil hcaplus

FILE 'HCAPLUS' ENTERED AT 17:32:02 ON 07 OCT 2000
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2000 AMERICAN CHEMICAL SOCIETY (ACS)


Copyright of the articles to which records in this database refer is
held by the publishers listed in the PUBLISHER (PB) field (available
for records published or updated in Chemical Abstracts after December
26, 1996), unless otherwise indicated in the original publications.

FILE COVERS 1967 - 7 Oct 2000  VOL 133 ISS 16
FILE LAST UPDATED: 6 Oct 2000  (20001006/ED)

 This file contains CAS Registry Numbers for easy and accurate
 substance identification.

 This file supports REG1stRY for direct browsing and searching of
 all substance data from the REGISTRY file.  Enter HELP FIRST for
 more information.

Now you can extend your author, patent assignee, patent information,
and title searches back to 1907.  The records from 1907-1966 now have
this searchable data in CAOLD.  You now have electronic access to all
of CA: 1907 to 1966 in CAOLD and 1967 to the present in HCAPLUS on STN.

=>

=>

=> d stat que l49 nos

L5              STR
L7         18360 SEA FILE=REGISTRY SSS FUL L5
L8              STR
L9          5204 SEA FILE=REGISTRY SUB=L7 SSS FUL L8
L10             STR
L11          484 SEA FILE=REGISTRY SUB=L9 SSS FUL L10
L12             STR
L14             STR
L17          988 SEA FILE=REGISTRY SSS FUL L12 AND L14
L18             STR
L19           60 SEA FILE=REGISTRY SUB=L17 SSS FUL L18
L20          418 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L11
L21           89 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L19
L23         5172 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L7
L24          895 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L17
L25            4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L23 AND L24
L27            1 SEA FILE=REGISTRY ABB=ON  PLU=ON  DNA/CN
L28               SEL  PLU=ON  L27 1- CHEM :        4 TERMS
L29       482681 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L28
L30       544802 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L29 OR DNA OR ?DEOXYRIBONU?
L31       528726 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L30 NOT (?DNASE? OR DNASE?)
L33            8 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20 AND ?NUCLEIC?(5A)ACID
L36           14 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20 AND (?PROTEIN? OR
                 AMINO(W)ACID OR AA OR ?PEPTID?)
L37           14 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L36 NOT (L25 OR L33)
L41           46 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L21 AND (L31 OR ?NUCLEIC? OR
                 ?PROTEIN? OR AMINO(W)ACID OR AA OR ?PEPTID?)
L42           46 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L41 NOT (L25 OR L33 OR L37)
L46          141 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ((L23 OR L24) AND L31) NOT
                 (L25 OR L33 OR L37 OR L42)
L48        72395 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L30(L)DETECT?
```

L49 10 SEA FILE=HCAPLUS ABB=ON PLU=ON L48 AND L46

=>

=>

=> d ibib abs hitrn 149 1-10

L49 ANSWER 1 OF 10 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 2000:188778 HCAPLUS
DOCUMENT NUMBER: 133:1821
TITLE: Orientation of Iron Bleomycin and Porphyrin Complexes on **DNA** Fibers
AUTHOR(S): Chikira, Makoto; Iiyama, Takamasa; Sakamoto, Katsuyuki; Antholine, William E.; Petering, David H.
CORPORATE SOURCE: Department of Applied Chemistry, Chuo University, Bunkyo-ku Tokyo, 112-8551, Japan
SOURCE: Inorg. Chem. (2000), 39(8), 1779-1786
CODEN: INOCAJ; ISSN: 0020-1669
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Bleomycin (Blm) is an antitumor agent that requires iron and oxygen for strand cleavage of **DNA**. In this study, ferric bleomycin, Fe(III)Blm, or the nitric oxide adduct of ferrous bleomycin, ON-Fe(II)Blm, were bound to one-dimensionally oriented **DNA** fibers. Reductive nitrosylation of Fe(III) complexes took place in situ on B-form **DNA** fibers. EPR spectra were obtained as a function of the angle .PHI. between the magnetic field B and the fiber axis Zf. For comparison, EPR spectra were acquired for ON-Fe(II)TMpyP and ON-Fe(II)TMpyP-Im on oriented **DNA** fibers, where TMpyP is 5,10,15,20-tetrakis(1-methyl-4-pyridino)porphyrin and Im is imidazole. EPR spectra showed both low-spin Fe(III)Blm and ON-Fe(II)Blm bound to B-form **DNA** in two slightly different binding orientations in the ratio of 1:0.2. With A-form **DNA**, a fraction of bound Fe(III)Blm was high spin. Specifically, the angle .beta. between the fiber axis Zf and the g axis, gz, perpendicular to or nearly perpendicular to the equatorial plane of the iron complex was estd. as 20.degree. and 25.degree. for ON-Fe(II)Blm and 30.degree. and 25.degree. for Fe(III)Blm, resp. The angle .gamma. that dets. the orientation of gx and gy axes was estd. as 90.degree. for the two ON-Fe(II)Blm species and 10.degree. for the two Fe(III)Blm species, resp. The NO was held rigidly in place as the temp. increased from 123 K to room temp. for ON-Fe(II)Blm but not for ON-Fe(II)TMpyP or ON-Fe(II)TMpyP-Im. It is hypothesized that the NO is structurally oriented by hydrogen bonding like the peroxide is held in HO2--Co(III)Blm (Wu et al. J. Am. Chem. Soc. 1996, 118, 1281-1294). The EPR parameters are consistent with a six-coordinate complex for ON-Fe(II)Blm, although the superhyperfine structure from the trans nitrogen was not **detected.** The increase in g value anisotropy upon binding ON-Fe(II)Blm to **DNA** fiber may be caused by an increase in the overlap of d.pi. and 2p.pi.* orbitals induced by an interaction of NO with **DNA** and/or by a perturbation of d orbitals due to the pyrimidine-guanine interaction. It is concluded that the EPR parameters of ON-Fe(II)Blm and Fe(III)Blm bound to oriented **DNA** support the hypothesis that FeBlm species bind to **DNA** with adduct structures similar to those formed by related CoBlm species and **DNA**.
IT **107985-26-2 270252-60-3**
RL: BPR (Biological process); PRP (Properties); BIOL (Biological study); PROC (Process)
(orientation of iron bleomycin and porphyrin complexes on **DNA** fibers)
REFERENCE COUNT: 58
REFERENCE(S): (1) Absalon, M; Biochemistry 1995, V34, P2076 HCAPLUS
(2) Akkerman, M; J Am Chem Soc 1990, V112, P7462

HCAPLUS
(3) Albertini, J; Biochemistry 1984, V23, P47 HCAPLUS
(4) Antholine, W; Biochem Biophys Res Commun 1979, V91, P528 HCAPLUS
(5) Barlow, C; FEBS Lett 1979, V98, P9 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 2 OF 10 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1999:725774 HCAPLUS
DOCUMENT NUMBER: 132:104221
TITLE: **DNA** cleavage by hydroxy-salicylidene-ethylendiamine-iron complexes
AUTHOR(S): Routier, Sylvain; Vezin, Herve; Lamour, Eric; Bernier, Jean-Luc; Catteau, Jean-Pierre; Bailly, Christian
CORPORATE SOURCE: Laboratoire de Chimie Organique Physique, URA CNRS 351, Villeneuve d'Ascq, 59655, Fr.
SOURCE: Nucleic Acids Res. (1999), 27(21), 4160-4166
CODEN: NARHAD; ISSN: 0305-1048
PUBLISHER: Oxford University Press
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Bis(hydroxy)salen.cntdot.Fe complexes were designed as self-activated chem. nucleases. The presence of a hydroxyl group on the two salicylidene moieties serve to form a hydroquinone system cooperating with the iron redox system to facilitate spontaneous formation of free radicals. We compared the **DNA** binding and cleaving properties of the ortho-, meta- and para-(bishydroxy) salen.cntdot.Fe complexes with that of the corresponding chelate lacking the hydroxyl groups. **DNA** melting temp. studies indicated that the para complex exhibits the highest affinity for **DNA**. In addn., this para compd. was considerably more potent at cleaving supercoiled plasmid **DNA** than the regio-isomeric ortho-and meta-hydroxy-salen.cntdot.Fe complexes, even in the absence of a reducing agent, such as dithiothreitol used to activate the metal complex. The **DNA** cleaving activity of the para isomer is both time and concn. dependent and the complexed iron atom is absolutely essential for the sequence uniform cleavage of **DNA**. From a mechanistic point of view, ESR measurements suggest that **DNA** contributes pos. to the activation of the semi-quinone system and the prodn. of ligand radical species responsible for subsequent strand scission in the absence of a reducing agent. The para-hydroxy-salen.cntdot.Fe complex has been used for **detecting** sequence-specific drug-**DNA** interactions. Specific binding of Hoechst 33258 to AT sequences and chromomycin to GC sequences were shown. The para-bis(hydroxy)salen.cntdot.Fe deriv. complements the tool box of footprinting reagents which can be utilized to produce efficient cleavage of **DNA**.
IT **255379-99-8**
RL: CAT (Catalyst use); NUU (Nonbiological use, unclassified); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(**DNA** binding and cleaving properties of ortho-, meta-, and para-(bishydroxy)salen.cntdot.Fe complexes)
IT **14167-12-5 93082-84-9 255379-97-6 255379-98-7**
RL: CAT (Catalyst use); PEP (Physical, engineering or chemical process); PROC (Process); USES (Uses)
(**DNA** binding and cleaving properties of ortho-, meta-, and para-(bishydroxy)salen.cntdot.Fe complexes)
REFERENCE COUNT: 23
REFERENCE(S): (1) Bailly, C; Biochemistry 1998, V37, P1033 HCAPLUS
(2) Britigan, B; J Biol Chem 1986, V261, P4426 HCAPLUS
(3) Burger, R; Chem Rev 1998, V98, P1153 HCAPLUS
(4) Burrows, C; Acc Chem Res 1994, V27, P295 HCAPLUS
(5) Canali, L; Chem Soc Rev 1999, V28, P85 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 3 OF 10 HCAPLUS COPYRIGHT 2000 ACS

ACCESSION NUMBER: 1999:157362 HCAPLUS
DOCUMENT NUMBER: 130:332464
TITLE: Structural variety of copper(II)-peroxide adducts and its relevance to **DNA** cleavage
AUTHOR(S): Nishino, Satoshi; Kobayashi, Teruyuki; Kunita, Mami; Ito, Sayo; Nishida, Yuzo
CORPORATE SOURCE: Inst. Molecular Sci., Okazaki, 444, Japan
SOURCE: Z. Naturforsch., C: Biosci. (1999), 54(1/2), 94-99
CODEN: ZNCBDA; ISSN: 0341-0382
PUBLISHER: Verlag der Zeitschrift fuer Naturforschung
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The reactivity of Cu(II) compds. with several tetradentate ligands towards some spin-trapping reagents was studied in the presence of H2O2. The compds. used in this study are roughly divided into 2 groups based on the reactivity towards 2,2,6,6-tetramethyl-4-piperidinol(and also 2,2,6,6-tetramethyl-4-piperidone), which are trapping agents for O, 1O2(1.DELTA.g); the A-group compds. exhibited a high activity to form the corresponding nitrone radical, which was **detected** by ESR spectroscopy, but corresponding activity of the B-group compds. was very low. The A-group compds. defined as above exhibited high activity for cleavage of **DNA** (supercoiled form I) in the presence of H2O2, yielding **DNA** form II (relaxed circular) or form III (linear duplex) under our exptl. conditions ([Cu(II)] = 0.1.apprx.0.5 mM). The B-group compds. effected complete degrdn. of the **DNA** (double-strand scission) under the same exptl. conditions, formation of form II or Form III **DNA** was negligible. 2 Different **DNA** cleavage patterns obsd. for A- and B-group compds. were elucidated by the different structural property of the Cu(II)-peroxide adducts, which is controlled by the interaction through both **DNA** and the peripheral group of the ligand system.

IT **209747-77-3**
RL: BPR (Biological process); BIOL (Biological study); PROC (Process)
(structural variety of Cu(II)-peroxide adducts and its relevance to **DNA** cleavage)

REFERENCE COUNT: 17
REFERENCE(S):
(4) Ito, S; Polyhedron 1998, V17, P1637 HCAPLUS
(5) Karlin, K; Inorg Chem 1982, V21, P4106 HCAPLUS
(7) Kobayashi, T; Polyhedron 1998, V17, P1553 HCAPLUS
(8) Lion, Y; Nature 1976, V263, P442 HCAPLUS
(9) McGall, G; J Am Chem Soc 1992, V114, P4958 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L49 ANSWER 4 OF 10 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1998:241359 HCAPLUS
DOCUMENT NUMBER: 129:38308
TITLE: Synthesis of metal complexes of 2,9-bis(2-hydroxyphenyl)-1,10-phenanthroline and their **DNA** binding and cleaving activities
AUTHOR(S): Routier, Sylvain; Joanny, Valerie; Zaparucha, Anne; Vezin, Herve; Catteau, Jean-Pierre; Bernier, Jean-Luc; Bailly, Christian
CORPORATE SOURCE: URA CNRS 351, USTL Bat. C3, Laboratoire de Chimie Organique Physique associe a l'ENSCL, Villeneuve d'Ascq, 59655, Fr.
SOURCE: J. Chem. Soc., Perkin Trans. 2 (1998), (4), 863-868
CODEN: JCPKBH; ISSN: 0300-9580
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

AB A series of metal complexes that combine the structure of phenanthroline and salen have been synthesized and characterized by ESR spectroscopy. The effects of the 2,9-bis(2-hydroxyphenyl)-1,10-phenanthroline compds. complexed with CuII, NiII, CoII, CoII or MnIII on the temp.-dependent helix-to-coil transition of **DNA** have been measured. The interaction with **DNA** is metal-dependent and the highest

stabilization is obsd. with the Co complex. The **DNA** cleaving activities have been studied with plasmid **DNA** and/or with a 32P-labeled duplex oligonucleotide depending on the redox properties of the complexes. The Cu complex is inactive whereas the Co chelate efficiency cleaves **DNA** in the presence of a reducing agent. Cleavage of **DNA** by the Mn complex can occur either in the presence of a reducing agent via the prodn. of oxygen radicals (which are **detected** by EPR spectroscopy) or in the presence of an oxidant such as KHSO5. In both cases, the cleavage of nucleic acids is very efficient whereas no cleavage is obsd. with the Ni complex. The complexes of bis(hydroxyphenyl)phenanthroline with Mn and Co complement the tool-box of reagents available for cleavage of **DNA**.

IT **192631-71-3P 192698-99-0P 208171-81-7P**
208171-82-8P
RL: SPN (Synthetic preparation); PREP (Preparation)
(synthesis of metal complexes of 2,9-bis(2-hydroxyphenyl)-1,10-phenanthroline and **DNA** binding and cleaving activities)

L49 ANSWER 5 OF 10 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1996:118313 HCAPLUS
DOCUMENT NUMBER: 124:225462
TITLE: Room temperature phosphorescent sensing probe for **detection** of **DNA**
AUTHOR(S): Diaz-Garcia, M.E.; Roza-Fernandez, M.
CORPORATE SOURCE: Faculty of Chemistry, University of Oviedo, Oviedo, 33006, Spain
SOURCE: Proc. SPIE-Int. Soc. Opt. Eng. (1995), Volume Date 1995, 2631, 29-36
CODEN: PSISDG; ISSN: 0277-786X
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The interaction between double-stranded **DNA** and a luminescent Pd-porphyrin complex was studied by room temp. phosphorescence (RTP). Intercalation of the Pd complex into **DNA** in deoxygenated soln. is accompanied by an obsd. enhanced RTP emission centered at 680 nm. Anal. of the RTP spectral data gave a value of 1.0 .times. 106 M-1 for the Pd complex-**DNA** assocn. const. and the complex seemed to bind **DNA** at the GC-rich environments. The spectroscopic features of this interaction and the anal. performance characteristics of the RTP method for **DNA** detn. are evaluated. The implication of the use of the Pd-complex RTP probe in combination with time-resolved luminescence measurements is discussed.

IT **171899-08-4**
RL: ARG (Analytical reagent use); ANST (Analytical study); USES (Uses)
(**DNA detection** by room-temp. phosphorescent sensing probe)

L49 ANSWER 6 OF 10 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1995:481943 HCAPLUS
DOCUMENT NUMBER: 122:208786
TITLE: Dynamics and Mechanism of the Exciplex Formation between Cu(TMpy-P4) and **DNA** Model Compounds Revealed by Time-Resolved Transient Absorption and Resonance Raman Spectroscopies
AUTHOR(S): Kruglik, Sergei G.; Galievsky, Victor A.; Chirvony, Vladimir S.; Apanasevich, Pavel A.; Ermolenkov, Vladimir V.; Orlovich, Valentine A.; Chinsky, Laurent; Turpin, Pierre-Yves
CORPORATE SOURCE: B. I. Stepanov Institute of Physics, Minsk, 220072, Belarus
SOURCE: J. Phys. Chem. (1995), 99(15), 5732-41
CODEN: JPCHAX; ISSN: 0022-3654
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The dynamics and mechanism of the photoinduced reversible process of formation and decay of an exciplex species created between the water-sol.

cationic metalloporphyrin copper 5,10,15,20-tetrakis[4-(N-methylpyridyl)]porphyrin (Cu(TMpy-P4)) and the **DNA** model compd. poly(dA-dT) have been studied in detail. Such a photoinduced process had been previously obsd. in transient resonance Raman (RR) spectra under high-power laser irradn. of complexes of Cu(TMpy-P4) with calf thymus **DNA** and some oligo- and polynucleotides contg. thymine (T) or uracil (U) residues. It was found that the interaction of excited Cu(TMpy-P4) with carbonyl groups of T or U involved in polymers having an appropriate secondary structure was responsible for the new transient species **detected** in high-power Raman spectra. In the present work, direct kinetic measurements of the exciplex formation between Cu(TMpy-P4) and poly(dA-dT) were carried out by using both picosecond transient absorption pump-probe technique (10-ps time resoln.) and two-color time-resolved RR technique (100-ps time resoln.). A comparative nanosecond Raman study of this exciplex and of the excited (d,d) state of copper meso-tetraphenylporphyrin (CuTPP) model compd. dissolved in a no. of oxygen-contg. solvents has also been performed, to clarify the excited electronic state which is at the origin of this process. It has been found that the binding of one of the CO-groups of T or U to Cu(TMpy-P4) in its lowest excited triplet state results in a shortening of the triplet-state lifetime to 35xb17 ps. In addn., a population of an excited 2[dz2,dx2-y2] state, i.e., the most low-lying and long-lived excited state for the five-coordinated Cu(TMpy-P4) (exciplex state), occurs in the process of excitation relaxation. Large wavenumber shifts of structure-sensitive vibrational marker lines from the porphyrin skeleton reveal the promotion of one of the copper d electrons into the half-filled dx2-y2 orbital and the expansion of the porphyrin core to accommodate the occupation of this d orbital. The exciplex deactivation process (excited (d,d) state decay) has a time const. of 3.2 .+-. 0.5 ns and is accompanied by the CO-group deattachment with a disruption of the exciplex into initial components.

IT **48242-70-2**, Copper 5,10,15,20-tetrakis[4-(N-methylpyridyl)]porphyrin
RL: RCT (Reactant)
(dynamics and mechanism of exciplex formation between Cu(TMpy-P4) and **DNA** model compds. revealed by time-resolved transient absorption and resonance Raman spectroscopies)

L49 ANSWER 7 OF 10 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1995:214243 HCAPLUS
DOCUMENT NUMBER: 122:26076
TITLE: Trans-Dioxorhenium(V)-Mediated Electrocatalytic Oxidation of **DNA** at Indium Tin-Oxide Electrodes: Voltammetric **Detection** of **DNA** Cleavage in Solution
AUTHOR(S): Johnston, Dean H.; Cheng, Chien-Chung; Campbell, Katherine J.; Thorp, H. Holden
CORPORATE SOURCE: Department of Chemistry, University of North Carolina at Chapel Hill, Chapel Hill, NC, 27599-3290, USA
SOURCE: Inorg. Chem. (1994), 33(26), 6388-90
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The oxidative electrochem. of trans-[Re(O)2(4-OMe-py)4]+ in the presence of **DNA** has been studied. The complex exhibits a reversible oxidn. at E1/2(VI/V) = 1.00 V (vs. Ag/AgCl) in buffer or in the presence of poly(dA).cntdot.poly(dT). However, in the presence of calf thymus **DNA** or poly(dG).cntdot.poly(dC), a dramatic catalytic enhancement is obsd. An identical result is obtained with Fe(5-Cl-phen)32+ (E1/2(III/II) = 1.02 V), but no electrocatalytic enhancement is obsd. with trans-[Re(O)2(py)2(dmap)2]+ (E1/2 = 0.90 V). Electrophoresis of plasmids electrolyzed at 1.2 V in the presence of trans-[Re(O)2(4-OMe-py)4]+ show relaxation from form I to form II, and analogous reactions with 5'-end 32P-labeled synthetic oligonucleotides show piperidine-labile cleavage specifically at guanine. The combined results point to an electrocatalytic mechanism where the oxidized metal complex oxidizes

guanine in **DNA** by one electron via an efficient, outer-sphere mechanism. Moreover, the expts. demonstrate a potential for the one-electron oxidn. of guanine in double-helical **DNA** at neutral pH of between 0.90 and 1.00 V. This result should provide insight into the mechanisms of **DNA** oxidn. by chem. agents and by ionizing radiation.

IT **94161-28-1**
RL: BSU (Biological study, unclassified); CAT (Catalyst use); PEP (Physical, engineering or chemical process); BIOL (Biological study); PROC (Process); USES (Uses)
(transdioxorhenium(V)-mediated electrocatalytic oxidn. of **DNA** at indium tin-oxide electrodes)

L49 ANSWER 8 OF 10 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1994:25734 HCAPLUS
DOCUMENT NUMBER: 120:25734
TITLE: Chemiluminescence investigation of the interaction of metalloporphyrins with nucleic acids
AUTHOR(S): Ci, Yun-Xiang; Zheng, Yuan-Gang; Tie, Jian-Ke; Chang, Wen-Bao
CORPORATE SOURCE: Department of Chemistry, Peking University, Beijing, 100871, Peop. Rep. China
SOURCE: Anal. Chim. Acta (1993), 282(3), 695-701
CODEN: ACACAM; ISSN: 0003-2670
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The interaction of water-sol. cationic porphyrin meso-tetrakis(4-N-methylpyridinyl)porphyrin (TMPyP) manganese derivs. with **DNA** was demonstrated by their catalytic activity on the luminol-H2O2 chemiluminescence (CL) system. The catalytic activity of Mn-TMPyP on the CL reaction was markedly enhanced when the complex was bound to **DNA**. The native form of **DNA** and thermally denatured **DNA** show the same degrees of enhancement. Different degrees of enhancement were obtained when Mn-TMPyP interacted with RNA and polynucleotides, whereas the interaction of nucleotides and bases with Mn-TMPyP had no effect on its catalytic activity. To examine the effect of the peripheral group of the porphyrin on its bonding properties, the interaction of manganese tetrakis(4-aminophenyl)porphyrin (Mn-TPPA4), manganese tetrakis(carboxylphenyl)porphyrin (Mn-TPPC4), manganese tetrakis(sulfophenyl)porphyrin (Mn-TPPS4) and manganese tetrakis(4-trimethylaminophenyl)porphyrin (Mn-TAPP) with **DNA** was tested. Only the Mn-TPPA4-catalyzed CL reaction was significantly enhanced. The effects of the native form of **DNA** and thermally denatured **DNA** on the Mn-TPPA4-catalyzed CL reaction were very different to that on the Mn-TMPyP-catalyzed CL reaction. With a fixed concn. of Mn-TMPyP there was a satd. concn. of **DNA** with respect to the metalloporphyrin (M-P). The binding no. of M-P to **DNA** was estd. Optimum conditions of the M-P-**DNA** complex-catalyzed luminol CL reaction were evaluated by using a flow-injection system. The use of the anal. parameters of the phenomenon as a means of detg. **DNA** was examd. The **detection** limit (signal-to noise ratio >3) of **DNA** was 0.20 ng mL-1. The relative std. deviation (n = 11) of the detn. of 10 ng mL-1 **DNA** was 2.6%.

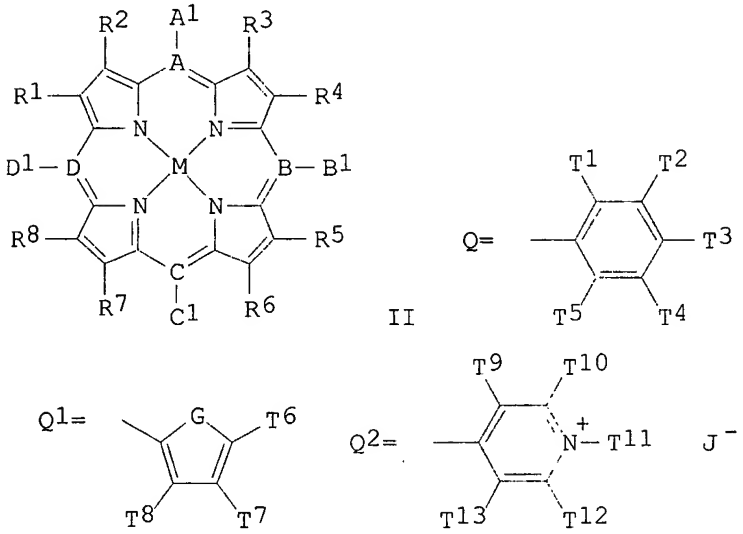
IT **72924-08-4**
RL: PRP (Properties)
(nucleic acids interactions with, chemiluminescence study of)

L49 ANSWER 9 OF 10 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1991:492309 HCAPLUS
DOCUMENT NUMBER: 115:92309
TITLE: Preparation of metal-porphyrin complexes catalyzing oxidation reaction as labeling agents for trace **detection** of **DNA** and proteins
INVENTOR(S): Ueno, Keihei; Sagara, Fumio; Shiga, Tadanobu
PATENT ASSIGNEE(S): Dojindo Laboratories, Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 03038587	A2	19910219	JP 1989-171372	19890703

OTHER SOURCE(S): MARPAT 115:92309
GI



AB The title compds. Z-[X-L-Y]n [I; Z = residue of metal-porphyrin represented by (II); A-D = sp2 C or N; R1-R8 = (CHR)kE, (CH:CH)kD; k = 0, 1; R = H, OH; E = H, CHO, CO2H, SO3H; R, E optionally being linked to X; or R1R2, R3R4, R5R6, R7R8 = benzene ring fused to the pyrrole ring; A1,B1,C1D1 = Q, Q1, Q2; T1-T13 = H, halo, alkyl; one of T1-T13 optionally being linked to X; G = O, S; J- = H-, MeSO2-, CF3SO3-, FSO3-, FSO3-, p-MeC6H4SO3-; M = Fe, Cr, Mn, Co, Ni, Cu, Zn, Mo, Cd, Os; X = linking group between II and a spacer L selected from NHCO, CONH, NHSO2, SO2NH, CO2, O2C, CH2, CH:CH, O, S, CO, CS, NH, N:CH, CH:N, C:NH, C:NOH; L = (CHR)m, (CH2CH2O)m, (OCH2CH2)m; Y = functional group bonding to proteins or nucleic acids or group convertible to the functional group] are prepd. Compds. such as proteins, oligopeptide, or **DNA** labeled with I catalyze oxidn. reaction with H2O2, perborate ion, or enzyme and can be **detected** in the presence of these oxidizing agents by (1) chemiluminescence in the copresence of a chemiluminescent agent, e.g. luminal derivs., and (2) formation of a dye in the copresence of an oxidative color coupler, e.g. aniline deriv. Thus, 6.71 pyrrole was added dropwise to a mixt. of Ac2O 11.3, 4-HO2CC6H4CHO 3.75, PhCHO 7.96, and 200 mL propionic acid at 120.degree. over 10 min and then resultant mixt. was heated at 20.degree. for 2 h to give, after purifn. by silica gel chromatog., .alpha.-(4-carboxyphenyl)-.beta.,.gamma.,.delta.-triphenylporphyrin (III), which (200 mg) was stirred with 90 mg FeCl3.cntdot.6H2O and 5 mg HgCl2 in 800 mL AcOH at 120.degree. for 16 h to give III.cntdot.Fe(III) complex. A soln. of 2.13 g the latter complex in THF/H2O(1:1) was stirred with 3.1 g dimethylaminopropylethylcarbodiimide hydrochloride at room temp. for 24 h to give .alpha.-(4-aminoethylcarbamoylphenyl)-.beta.,.gamma.,.delta.-triphenylporphynate-Fe(III)(IV). IV was condensed with .gamma. phage **DNA** and glutaraldehyde in H2O to give IV-labeled .lambda. phage **DNA**

which was **detected** at a 10 pg level by chemiluminescence produced from H2O2 and luminol, on an polaroid instant film 612. A total of 20 I were prepd.

IT **135364-25-9P**
RL: SPN (Synthetic preparation); PREP (Preparation)
(prepn. of, as labeling agent for trace **detection** of **DNA** and proteins)

L49 ANSWER 10 OF 10 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1990:231408 HCAPLUS
DOCUMENT NUMBER: 112:231408
TITLE: On the chemical nature of **DNA** and RNA modification by a hemin model system
AUTHOR(S): Van Atta, Reuel B.; Bernadou, Jean; Meunier, Bernard; Hecht, Sidney M.
CORPORATE SOURCE: Dep. Chem., Univ. Virginia, Charlottesville, VA, 22901, USA
SOURCE: Biochemistry (1990), 29(20), 4783-9
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB In order to model the interaction of hemin with **DNA** and other polynucleotides, the degrdn. of **DNA**, RNA, and polynucleotides of defined structure by [meso-tetrakish(N-methyl-4-pyridyl)porphinato]manganese(III) (MnTMPP) + KHSO5 was studied. The activated porphyrin released adenine, thymine, and cytosine from **DNA**; RNA degrdn. afforded adenine, uracil, and cytosine. The same products were obtained from single- and double-stranded **DNA** oligonucleotides of defined sequence, and also from single-stranded **DNA** and RNA homopolymers. The overall yield of bases from the dodecanucleotide d(CGCT3A3GCG) was equal to 14% of the nucleotides present initially, indicating that each porphyrin catalyzed the release of .apprx.4 bases. Although no guanine (G) was **detected** as a product from any of the substrates studied, the ability of NmTMPP + KHSO5 to degrade guanine nucleotides was verified by the destruction of pGp, and by the appearance of bands corresponding to guanosine cleavage following treatment of 32P end-labeled **DNA** restriction fragments with activated MnTMPP. Inspection of a no. of sites of MnTMPP-promoted cleavage indicated that the process was sequence-selective, occurring primarily at G residues that were part of 5'-TG-3' or 5'-AG-3' sequences, or at T residues. Also formed in much greater abundance were alkali-labile lesions; these were formed largely at guanosine residues. Also studied was the degrdn. of a 47-nucleotide RNA mol. contg. 2 hairpins. Degrdn. of the 5'-32P end labeled RNA substrate afforded no distinct, individual bands, suggesting that multiple modes of degrdn. may be operative. However, at concns. of MnTMPP + KHSO5 that led to only limited amts. of RNA substrate degrdn., there was enhanced degrdn. in a single-stranded region between the 2 hairpins, suggesting that MnTMPP may be a useful probe of RNA conformation.

IT **110989-01-0**
RL: BIOL (Biological study)
(nucleic acid degrdn. by oxone and, as hemin model system)

=> d stat que l51 nos

```
L5              STR
L7        18360 SEA FILE=REGISTRY SSS FUL L5
L8              STR
L9         5204 SEA FILE=REGISTRY SUB=L7 SSS FUL L8
L10             STR
L11         484 SEA FILE=REGISTRY SUB=L9 SSS FUL L10
L12             STR
L14             STR
L17         988 SEA FILE=REGISTRY SSS FUL L12 AND L14
L18             STR
```

```
L19          60 SEA FILE=REGISTRY SUB=L17 SSS FUL L18
L20         418 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L11
L21          89 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L19
L23        5172 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L7
L24         895 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L17
L25           4 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L23 AND L24
L27           1 SEA FILE=REGISTRY ABB=ON  PLU=ON  DNA/CN
L28             SEL  PLU=ON  L27 1- CHEM :        4 TERMS
L29      482681 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L28
L30      544802 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L29 OR DNA OR ?DEOXYRIBONU?
L31      528726 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L30 NOT (?DNASE? OR DNASE?)
L33           8 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20 AND ?NUCLEIC?(5A)ACID
L36          14 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L20 AND (?PROTEIN? OR
                AMINO(W)ACID OR AA OR ?PEPTID?)
L37          14 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L36 NOT (L25 OR L33)
L41          46 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L21 AND (L31 OR ?NUCLEIC? OR
                ?PROTEIN? OR AMINO(W)ACID OR AA OR ?PEPTID?)
L42          46 SEA FILE=HCAPLUS ABB=ON  PLU=ON  L41 NOT (L25 OR L33 OR L37)
L46         141 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ((L23 OR L24) AND L31) NOT
                (L25 OR L33 OR L37 OR L42)
L50      196525 SEA FILE=HCAPLUS ABB=ON  PLU=ON  (?NUCLEIC? OR ?PROTEIN? OR
                AMINO(W)ACID OR AA OR ?PEPTID?)(L)DETECT?
L51           7 SEA FILE=HCAPLUS ABB=ON  PLU=ON  ((L23 OR L24) AND L50) NOT
                (L25 OR L33 OR L37 OR L42 OR L46)


=>

=>

=> d ibib abs hitrn l51 1-7


L51  ANSWER 1 OF 7  HCAPLUS  COPYRIGHT 2000 ACS
ACCESSION NUMBER:         2000:385416  HCAPLUS
DOCUMENT NUMBER:          133:199326
TITLE:                    Kinetics and mechanism of formation, acid catalyzed
                          aquation, reversible anation and photochemical
                          reaction of trans-(aqua)(sulfito-S
                          )[N,N'-ethylenebis(salicylidiniminato)]cobaltate(III)
                          in aqueous media
AUTHOR(S):                Das, Arabinda; Dash, Anadi C.
CORPORATE SOURCE:         Department of Chemistry, Utkal University,
                          Bhubaneswar, 751 004, India
SOURCE:                   Dalton (2000), (12), 1949-1958
                          CODEN: DALTFG
PUBLISHER:                Royal Society of Chemistry
DOCUMENT TYPE:            Journal
LANGUAGE:                 English
AB   The reaction of trans-[Co(salen)(OH2)OH] with SO2 yields
     trans-[Co(salen)(OH2)(SO3-S )]- (S-bonded isomer) for which the rate and
     activation parameters at 25 .degree.C (I = 0.3 mol dm-3) are kSO.degree.2
     = (5.9 .+-. 0.1) .times. 1010 dm3 mol-1 s-1, .DELTA.H .dbldag. = 66 .+-. 4
     kJ mol-1 and .DELTA.S .dbldag. = 183 .+-. 14 J K-1 mol-1.  One possibility
     for the SIV substitution is that Co-S bond formation is concerted with
     Co-O bond breaking.  An alternative mechanism, involving a fast equil.
     between SO2 and trans-[Co(salen)(OH2)OH] forming an O-bonded sulfito
     species which then undergoes sulfite ligand linkage isomerization, is also
     possible.  An estd. value of the isomerization rate const. for the
     trans-[Co(salen)(OH2)(OSO2H)] at 25 .degree.C is ca. 106 s-1.  The
     trans-[Co(salen)(OH2)(SO3-S )]- (pK = 10.1 .+-. 0.1 at 25 .degree.C, I =
     0.3 mol dm-3) undergoes acid catalyzed aquation to yield the parent diaqua
     complex and SIV with kH = 29.5 .+-. 1.1 dm3 mol-1 s-1, .DELTA.H .dbldag. =
     72 .+-. 3 kJ mol-1, .DELTA.S .dbldag. = 24 .+-. 9 J K-1 mol-1 at 25
     .degree.C (I = 0.3 mol dm-3).  Steady state photolysis (254 nm) of
     trans-[Co(salen)(OH2)(SO3-S )]- resulted in the redn. of CoIII. The redox
```

rate const. and .phi.(Co2+) decreased with increasing pH. Attempts to **detect** an O-bonded sulfito complex as a transient in the conventional flash photolysis of this aqua-sulfito complex proved unsuccessful. The aqua ligand replacement reactions of trans-[Co(salen)(OH2/OH)(OH2)]+/0 with imidazole and that of the corresponding aqua-sulfito complex with N3-, NCS-, imidazole, and SIV in a large excess of the entering ligands have been studied at 25 .degree.C. A comparison of the rate consts. with the analogous data for trans-[Co(**AA**)2(OH2)(SO3-S)]+ (**AA** = 1,2-diaminoethane; 1,3-diaminopropane) clearly shows that the kinetic trans-effect of the S-bonded sulfite is substantially attenuated in trans-[Co(salen)(OH2)(SO3-S)]-.

IT **289058-25-9**
RL: FMU (Formation, unclassified); PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); FORM (Formation, nonpreparative); PROC (Process)
(kinetics and mechanism of formation, acid catalyzed aquation, reversible anation and photochem. reaction of trans-(aqua)(sulfito-S)[N,N'-ethylenebis(salicylidiniminato)]cobaltate(III) in aq. media)

IT **21710-17-8 33569-62-9**
RL: PEP (Physical, engineering or chemical process); PRP (Properties); RCT (Reactant); PROC (Process)
(kinetics and mechanism of formation, acid catalyzed aquation, reversible anation and photochem. reaction of trans-(aqua)(sulfito-S)[N,N'-ethylenebis(salicylidiniminato)]cobaltate(III) in aq. media)

REFERENCE COUNT: 46
REFERENCE(S):
(1) Acharya, A; Proc Indian Acad Sci (Chem Sci) 1993, V105, P225 HCAPLUS
(2) Ali, M; J Chem Soc, Dalton Trans 1990, P187 HCAPLUS
(6) Boyce, S; Environ Sci Technol 1983, V17, P602 HCAPLUS
(7) Brandt, C; Chem Rev 1995, V95, P119 HCAPLUS
(8) Brandt, C; Inorg Chem 1994, V33, P687 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 2 OF 7 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1999:326416 HCAPLUS
DOCUMENT NUMBER: 131:195581
TITLE: Hydroxopentaamminechromium(III) promoted phosphorylation of bovine serum albumin: its potential implications in understanding biotoxicity of chromium
AUTHOR(S): Balamurugan, Kuppusamy; Vasant, Chellappa; Rajaram, Rama; Ramasami, Thirumalachari
CORPORATE SOURCE: Chemical Laboratory, Central Leather Research Institute, Chennai, India
SOURCE: Biochim. Biophys. Acta (1999), 1427(3), 357-366
CODEN: BBACAQ; ISSN: 0006-3002
PUBLISHER: Elsevier Science B.V.
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Evidence for chromium(III) induced phosphorylation of a biomarker **protein** bovine serum albumin (BSA) is presented. Radiolabeled ATP was reacted with BSA in the presence of various Cr(III) salts. While [Cr(NH3)5(H2O)]3+ brought about phosphorylation of BSA, several Cr(III) complexes, viz. [Cr(bpy)3]3+, [Cr(phen)3]3+, [Cr(en)3]3+, [Cr(salen)(H2O)2]+ and [Cr(salprn)(H2O)2]+, did not phosphorylate BSA. The Cr(III) mediated the transfer of .gamma.- and .alpha.-phosphates but not the adenine and the sugar moieties of the ATP mol. to BSA. The obsd. stoichiometry was 0.75 mol Pi to mol. BSA for the .gamma.-phosphate and 0.5 mol Pi to mol. BSA for the .alpha.-phosphate of ATP. The presence of serine phosphate and threonine phosphate was **detected** in the hydrolyzate of phosphorylated BSA by means of comparison of Rf values with authentic samples of phosphoserine and phosphothreonine after chromatog. sepn. and autoradiog. [Cr(NH3)5(H2O)]3+ at pH 7.4 is known to exist as the conjugate base [Cr(NH3)5(OH)]2+ and is capable of ligand substitution

involving metal-oxygen bond retention. Such anation reaction of [Cr(NH3)5(OH)]2+ with ATP subsequently leads to the esterification of alc. hydroxyl groups of serine and threonine of BSA. Possible consequences of chromium(III) induced in vivo phosphorylation of **proteins** are discussed.

IT **98672-30-1**
RL: ADV (Adverse effect, including toxicity); BIOL (Biological study)
(hydroxopentaamminechromium(III) promoted phosphorylation of serum albumin in relation to toxicity of chromium)

REFERENCE COUNT: 31
REFERENCE(S):
(4) Blithe, D; J Biol Chem 1982, V257, P7135 HCAPLUS
(5) Cheng, Y; Proc Natl Acad Sci 1981, V78, P2388 HCAPLUS
(7) Cohen, P; Nature 1982, V296, P613 HCAPLUS
(8) Coogan, T; Toxicol Appl Pharmacol 1991, V109, P60 HCAPLUS
(9) Kane-Maguire, N; Inorg Chim Acta 1979, V35, PL309 HCAPLUS
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L51 ANSWER 3 OF 7 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1999:255594 HCAPLUS
DOCUMENT NUMBER: 130:346455
TITLE: Optical fiber sensing for copper ion using a polyvinyl chloride membrane containing chelating reagent as a detection port
AUTHOR(S): Shimizu, Yuuzi; Saito, Takashi
CORPORATE SOURCE: Department of Applied Chemistry, Kanagawa Institute of Technology, Atsugi-shi, Kanagawa, 243-0292, Japan
SOURCE: Bunseki Kagaku (1999), 48(4), 429-433
CODEN: BNSKAK; ISSN: 0525-1931
PUBLISHER: Nippon Bunseki Kagakkai
DOCUMENT TYPE: Journal
LANGUAGE: Japanese

AB The **detection** of a copper ion by an optical fiber sensing system using a polyvinyl chloride (PVC) membrane contg. N,N'-bissalicyliden-2,3-diaminobenzofuran (SABF) as a **detection** port is discussed. A PVC membrane contg. SABF and dioctylphthalate (DOP) was prepd. and attached to the sensor port of an optical fiber sensor. A copper ion sample soln. was added a 5 .times. 10-2 mol dm-3 counterion solns. and a pH 6 buffer soln. Then, a sensor fixed in order PVC membrane was soaked in the sample soln. The absorbance of the colored membrane was measured by a spectrophotometer at 530 nm. The **detectable** concn. of the copper ion detd. by the proposed method was over the range of 10-6-10-3 mol dm-3, and the reproducibility of the detd. values of the copper ion was 2.0% as a relative std. deviation on repeatable expts. (six times) for 10-4 mol dm-3 of the copper ion sample. A linear correlation between the detd. values by the proposed method and those by **AAS** was obtained over a concn. range of 1 x 10-5 .apprx. 1 x 10-4 mol dm-3. Coexisting metal ions had almost no effect on the detd. values of copper ion. However, when zinc, nickel and magnesium ions coexisted with copper ions, it brought about neg. interference to the detd. values of copper ion.

IT **27295-38-1**
RL: ANT (Analyte); FMU (Formation, unclassified); ANST (Analytical study); FORM (Formation, nonpreparative)
(copper ion detn. in aq. soln. by fiber optic sensor based on polyvinyl chloride membrane contg. N,N'-bissalicyliden-2,3-diaminobenzofuran)

L51 ANSWER 4 OF 7 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1998:173457 HCAPLUS
DOCUMENT NUMBER: 128:291233
TITLE: Peroxynitrite decomposition catalysts: therapeutics for peroxynitrite-mediated pathology
AUTHOR(S): Salvemini, Daniela; Wang, Zhi-Qiang; Stern, Michael K.; Currie, Mark G.; Misko, Thomas P.

CORPORATE SOURCE: Discovery Pharmacology, G. D. Searle Co, St. Louis, MO, 63167, USA
SOURCE: Proc. Natl. Acad. Sci. U. S. A. (1998), 95(5), 2659-2663
CODEN: PNASA6; ISSN: 0027-8424
PUBLISHER: National Academy of Sciences
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Inflamed tissue is often characterized by the prodn. of NO and superoxide. These radicals react at diffusion-limited rates to form the powerful oxidant peroxynitrite (PN). When protonated, PN decomps. into either nitrate or reactive intermediates capable of mediating tissue damage by oxidn. of **protein**, lipid, and **nucleic** acid. The authors recently have identified porphyrin derivs. capable of catalyzing an increase in nitrate formation with a concomitant decrease in the HO.bul.-like and NO2.bul.-like reactivity of PN. Here, we present evidence for the efficacy of these PN decompn. catalysts both in vitro and in vivo. Cells in culture were protected from exogenously added PN by the catalyst 5,10,15,20-tetrakis(2,4,6-trimethyl-3,5-disulfonatophenyl)porphyrinato iron (III), whereas free iron and the structurally related compd. without iron 5,10,15,20-tetrakis(2,4,6-trimethyl-3,5-disulfonatophenyl)porphyrin did not protect. Cytoprotection correlated well with a redn. in the nitrotyrosine content of released cytosolic **proteins**, a biochem. marker for PN formation. Carrageenan-induced paw edema is a model of acute inflammation in which PN may play a major role. When tested in this system, both 5,10,15,20-tetrakis(2,4,6-trimethyl-3,5-disulfonatophenyl)porphyrinato iron (III) and 5,10,15,20-tetrakis(N-methyl-4'-pyridyl)porphyrinato iron (III) caused a dose-dependent redn. in swelling and lactate dehydrogenase release as well as a **detectable** shift to nitrate formation in paw tissue. In addn., the catalysts did not elevate mean arterial pressure, suggesting a lack of interaction with NO. Taken together, our data provide compelling evidence supporting the therapeutic value of manipulating PN pharmacol. Thus, PN decompn. catalysts may represent a unique class of anti-inflammatory agents.

IT **60489-13-6**, 5,10,15,20-Tetrakis(N-methyl-4'-pyridyl)porphyrinato iron(III)
RL: BAC (Biological activity or effector, except adverse); BIOL (Biological study)
(peroxynitrite decompn. catalysts and therapeutics for peroxynitrite-mediated pathol.)

L51 ANSWER 5 OF 7 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1993:554734 HCAPLUS
DOCUMENT NUMBER: 119:154734
TITLE: Model studies of catechol dioxygenases. Important role of monodentate catecholate-iron(III) intermediate
AUTHOR(S): Fujii, Satoshi; Ohya-Nishiguchi, Hiroaki; Hirota, Noboru; Nishinaga, Akira
CORPORATE SOURCE: Fac. Sci., Kyoto Univ., Kyoto, 606, Japan
SOURCE: Bull. Chem. Soc. Jpn. (1993), 66(5), 1408-19
CODEN: BCSJA8; ISSN: 0009-2673
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The catechol dioxygenase model reactions of 3 model systems were investigated by EPR, optical, and electrochem. studies. In each model system, some kinds of intermediates could be **detected** by EPR and optical spectroscopies. The intermediate structures and the reaction times suggested that the monodentate catecholate complexes play an important role in the catalytic cycle. Based on the EPR spectra obtained aerobically and anaerobically, Fe(III)-monodentate dianionic catecholate is the O2-reactive species for the Fe-(nta) (nta = nitrilotriacetato) and Fe(sal-L-**aa**)Cl (sal-L-**aa** = N-salicylidene L-amino acidato) systems and Fe(II)-semiquinonate for the Fe(salen)Cl (salen = N,N'-ethylenebis(salicylideneaminato) system. Electrochem. data suggested that this electron transfer in the Fe(salen)Cl system is caused by ligand

distortion. The catecholate(sal-L-val)-Fe(III) complex reacted with O2 to yield the ring cleavage products (.apprx.80%). On the basis of the observations, the novel reaction mechanism of the Fe(sal-L-**aa**)Cl system having mainly monodentate catecholate intermediate, was proposed. Finally, the correlation between the coordination environments of nonheme Fe(III) complexes and EPR parameters was discussed.

IT **78165-60-3**
RL: PRP (Properties)
(absorption and ESR spectra of, as catechol dioxygenase model)

L51 ANSWER 6 OF 7 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1993:32372 HCAPLUS
DOCUMENT NUMBER: 118:32372
TITLE: Flow injection and liquid chromatographic postcolumn **detection** of **amino acids** by mimetic peroxidase-catalyzed chemiluminescence reaction
AUTHOR(S): Ci, Yunxiang; Tie, Jianke; Wang, Qinwei; Chang, Wenbao
CORPORATE SOURCE: Dep. Chem., Beijing Univ., Beijing, 100871, Peop. Rep. China
SOURCE: Anal. Chim. Acta (1992), 269(1), 109-14
CODEN: ACACAM; ISSN: 0003-2670
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Four **amino acids** were detd. on the basis of the finding that the catalytic activity of mimetic peroxidase (metalloporphyrin) in the chemiluminescence reaction between luminol and hydrogen peroxide is inhibited in the presence of an **amino acid**. The degree of chemiluminescence inhibition is a measure of the **amino acid** concn. The electrostatic interaction between **amino acid** and metalloporphyrin was confirmed by comparing the degree of inhibition of cationic and anionic metalloporphyrin-catalyzed chemiluminescence reactins. More than 20 **amino acids** were tested, and only L-cysteine, L-tyrosine, L-tryptophan and L-cystine significantly quenched the chemiluminescence intensity. The **detection** limits were 6.8 x 10-8, 1.3 x 10-7, 8.5 x 10-6 and 2.2 x 10-5M, resp. The **detection** approach is demonstrated with a silica-based liq. chromatog. sepn. of **amino acids** using phosphate buffer (pH 7.3) as mobile phase. Compared with other chemiluminescence analyses, this method is faster, can be run at room temp. and, in favorable cases, has a lower **detection** limit.

IT **71794-64-4**
RL: ANST (Analytical study)
(luminol/hydrogen peroxide chemiluminescence catalyzed by, **amino acid detection** based on inhibition effect on)

L51 ANSWER 7 OF 7 HCAPLUS COPYRIGHT 2000 ACS
ACCESSION NUMBER: 1991:177147 HCAPLUS
DOCUMENT NUMBER: 114:177147
TITLE: Structural studies of metalloporphyrins. 10. Complexes of water-soluble cobalt(III) porphyrins with amino acids: NMR study of the conformation of the complexes with cobalt(III) tetrakis[4-(N-methylpyridiniumyl)]porphine (CoTMPyP) and cobalt(III) tetrakis(4-carboxylatophenyl)porphine (CoTCPP)
AUTHOR(S): Mikros, Emmanouil; Gaudemer, Francoise; Gaudemer, Alain
CORPORATE SOURCE: Inst. Chim. Mol., Univ. Paris-Sud, Orsay, F-91405, Fr.
SOURCE: Inorg. Chem. (1991), 30(8), 1806-15
CODEN: INOCAJ; ISSN: 0020-1669
DOCUMENT TYPE: Journal
LANGUAGE: English

AB [CoQL2] (H2Q = tetrakis(4-N-methylpyridiniumyl)porphine tetrachloride (H2TMPyP) or tetrasodium tetrakis(4-carboxylatophenyl)porphine (H2TCPP)

and HL = **amino acid**)) were studied in H2O soln. by 1H NMR spectroscopy. [CoQL2]- are the predominant species at pH > 7, whereas at lower pH values CoQL(H2O) are also present. In the general case, the 2 **amino acid** ligands were bound to the Co atom through the NH2 group. In the case of histidine, 3 different complexes with Co(TMPyP), 2 sym. and 1 unsym., were **detected** in proportions that varied with the pH of the soln.: at pH 7, histidine was bound to Co exclusively through imidazole N-3, and at pH > 10, it was bound only through the NH2 group. Similar behavior was found for methionine and lysine. The predominant species at pH 10 were the NH2-bound complexes, in both cases. The conformational anal. of these complexes was performed by using 2 sets of NMR data, the vicinal interproton coupling consts., JNH-H.alpha., JH.alpha.-H.beta., and JH.beta.-H.alpha., and the induced shifts, .DELTA..delta.. All **amino acids** studied adopt a largely predominant geometry characterized by a nearly eclipsed conformation around the N-C.alpha. bond and conformation I around C.alpha.-C.beta.. This geometry allows the side chain of the **amino acid** to interact with the porphyrin macrocycle by either stacking (arom. **amino acids**), hydrophobic (e.g. leucine), or electrostatic (e.g. aspartic acid) interactions. Existence of the last interactions were confirmed by the conformational anal. of the complexes of the same **amino acids** with Co(TCPP), which revealed that only the polar **amino acids** aspartic acid, serine, and asparagine had different geometries in the 2 types of complexes. Comparison of the const. K for the open form .tautm. closed form equil. in the free and complexed **amino acids** showed that the gain of stability -.DELTA..DELTA.G.degree. of the closed form upon complexation increases in the order His < TyrO- < Phe < TyrOH < Trp. Temp. dependence of .DELTA..DELTA.G.degree. values indicates that the enthalpy change contributes to the stabilization due to the stacking interaction in the case of the arom. **amino acids**.

IT **133100-49-9P 133100-50-2P 133100-51-3P**
133100-52-4P 133100-53-5P 133100-54-6P
133100-55-7P 133100-56-8P 133100-57-9P
133100-58-0P 133100-59-1P 133100-60-4P
133100-61-5P 133100-62-6P 133100-63-7P
133100-64-8P 133100-65-9P 133100-66-0P
133100-67-1P 133100-68-2P 133100-69-3P
133100-70-6P 133128-02-6P 133128-03-7P
RL: FORM (Formation, nonpreparative); PREP (Preparation)
(formation of, NMR study of)

IT **98938-65-9**
RL: RCT (Reactant)
(reactions of, with amino acids, NMR study of)

=>

=>

=> select hit rn 149 1-10;select hit rn 151 1-7

E37 THROUGH E54 ASSIGNED

E55 THROUGH E87 ASSIGNED

=> fil reg

FILE 'REGISTRY' ENTERED AT 17:36:48 ON 07 OCT 2000
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

STRUCTURE FILE UPDATES: 6 OCT 2000 HIGHEST RN 293726-17-7
DICTIONARY FILE UPDATES: 6 OCT 2000 HIGHEST RN 293726-17-7